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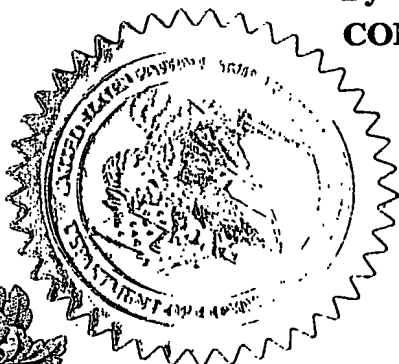
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PART (1) OF 3 PART(S)

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IN THE UNITED STATES PATENT AND TRADEMARK OFFICE

Applicant: Francois Andre et al.

Title: A METHOD FOR PERFORMING RESTRAINED
DYNAMICS DOCKING OF ONE OR MULTIPLE
SUBSTRATES ON MULTI-SPECIFIC ENZYMES

Appl. No.: Unknown

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Sir:

Transmitted herewith for filing under 37 C.F.R. § 1.53(c) is the provisional patent
application of:

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Enclosed are:

- ☒ Specification, Claim(s), and Abstract (761 pages).
- ☒ Informal drawings (7 sheets, Figures 1-5).
- ☒ Application Data Sheet (37 CFR 1.76).

The filing fee is calculated below:

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- ☒ A check in the amount of \$160.00 to cover the filing fee is enclosed.
- ☒ Further, Applicant, by and through his attorney of record, hereby expressly abandons the application as of the filing date of this letter. This is an abandonment of the application only, and is not to be construed as an abandonment of the invention disclosed in the application. It is respectfully requested that the Office acknowledge abandonment of the application as of the filing date of this letter in a communication mailed to the undersigned.
- ☒ The Commissioner is hereby authorized to charge any additional fees which may be required regarding this application under 37 C.F.R. §§ 1.16-1.17, or credit any overpayment, to Deposit Account No. 19-0741. Should no proper payment be enclosed herewith, as by a check being in the wrong amount, unsigned, post-dated, otherwise improper or informal or even entirely missing, the Assistant Commissioner is authorized to charge the unpaid amount to Deposit Account No. 19-0741.

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Application Data Sheet

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 FRACTIONNEMENT ET DES
 BIOTECHNOLOGIES

A method for performing restrained dynamics docking of one or multiple substrates on multi-specific enzymes

5 The present invention relates to a method for performing restrained dynamics docking of one or several substrates having allosteric or synergistic effect on enzymes presenting multispecific and flexible active site. It also concerns a method for determining the 3D-structure of active sites that are flexible and can adapt to different substrates, which is the case for multispecific enzymes such as cytochrome
10 P450.

Background

As of today, various computer graphics systems allow to generate molecular models
15 of large molecules such as proteins from the PDB structural data obtained using X-ray crystallography and NMR. We can cite for example MODELLER, MATCHMAKER (Tripos), or 3D graphical environments for molecular modeling such as SYBYL (Tripos) or INSIGHT II (Accelrys).

20 Substrates as well as inhibitors or agonists often act by binding to particular regions of an enzyme or receptor referred as the active site. In industry, the purpose of using these 3D models is to assess the main features of the molecules which are involved in the binding to the active site. New molecules that fit the active site can be designed.

25 Biological interactions are not possible without flexibility and motion. The molecular dynamics simulations which recreate the successive events in the binding process of a molecule and thermodynamic parameters implicated in such process is therefore of great interest in the design of active molecules.

30 Nevertheless, the methods proposed in the art are based on a relatively low level of calculations of few parameters. It relies only on the molecule energy constrained

with a fixed geometry. It relies only on the interaction energy between the molecule and the active site frozen in a fixed geometry

Consequently, there is a need for a model replicating *in silico* the natural process of molecular interactions.

The method according to the invention provides both minimizations and molecular dynamics calculations. More specifically, it provides a new approach which is more appropriate to flexible structures, hereafter referred as "restrained dynamics docking" or "soft-restrained restrained dynamics docking". This technique employs constrained dynamics simulations, where the only constraints are active site-substrate distances.

For example, to explain and predict drug metabolism in organisms, in which the cytochrome P450 (CYP) superfamily of haem-thiolate enzymes plays a central role, it is of large interest to dispose of a molecular picture of the binding sites responsible for the biotransformation. Efficiency of the prediction is then directly related to the molecular precision of the model, which resolution must be obtained at the atomic level to exploit the model for further docking studies.

20

In mammalian, hepatic cytochrome P450s constitute the major enzymes involved in the metabolism of exogenic compounds. Among them, isozymes of the CYP3 family (such as CYP3A1 and 3A2 in rat, and CYP3A4 in human) are known to metabolize the majority of drugs in clinical use. These are multi-specific enzymes, able to metabolize a large variety of structurally diverse chemicals, generally fairly lipophilic, within a broad range of molecular sizes from testosterone (Mw 288) to cyclosporin A (Mw 1203). Consequently, any molecular model describing correctly the multiple substrate specificity (that takes into account large variations in molecular size and chemical structures), and substrate cooperativity effects within the active site (when two or more drugs interact), is of considerable scientific and industrial interest. Such a molecular model must be able to rationalize the binding of the diverse known substrates, and the orientations of the molecules in the binding

site that account for their known positions of metabolism (such as N-demethylations, benzylic hydroxylations etc.).

As no high-resolution 3D structure of CYP3A is today publicly available, due to continuing difficulties in promoting crystallization of intrinsic membrane proteins or due to an unusual conformational flexibility that would explain how CYP3A4 can accommodate various substrates, it is necessary to rebuild a 3D model structure, integrating the known biochemical data of CYP3A4 and the structural data of other members of the CYP superfamily. X-ray crystallographic determinations of several bacterial P450 enzymes in the 1990s (see table 1 for a summary of structural data) have stimulated numerous attempts in modeling microsomal P450S such as human CYP3A4. The chapter 6 of the book "Guide to Cytochromes P450: structure and function" written by David F.V. Lewis reviews the current status of structural and modeling investigations of the P450 family (Lewis 2001). This review was however written just before the release of the first mammalian P450 structure (2C5), still today the only one mammalian template available.

Table 1

CYP isoform crystallized	PDB code (resol.)	Organism	Function	No of residues	Reference
P450 cam (complexed by CO+camphor)	3cpp (1.9 Å)	<i>Pseudomonas Putida</i>	Camphor Monooxygenase	414	(Poulos et al. 1985) (Raag and Poulos 1989)
P450 terp	1cpt (2.3 Å)	<i>Pseudomonas</i> sp.	Alpha-terpineol hydroxylation	412	(Hasemann et al. 1994)
P450 BM3	2hpd (2 Å)	<i>Bacillus megaterium</i>	Fatty acid monooxygenase	471	(Ravichandran et al. 1993)
P450 eryF (6-deoxyerythronolide B bond)	1oxa (2.1 Å)	<i>Saccharopolyspora erythraea</i>	Erythromycin biosynthesis 6S-hydroxylation of 6-deoxyerythronolide B	403	(Cupp-Vickery and Poulos 1995)
P450 nor	1rom (2 Å)	<i>Fusarium oxysporum</i> (denitrifying fungus)	Nitric Oxide Reductase	403	(Park et al. 1997)
P450 2C5	1dt6 (3 Å)	(membrane-type Mammalian) Rabbit	Progesterone 21-Hydroxylase	489	(Williams et al. 2000)
P450 CYP119 4-Phenylimidazole	1f4t (1.93 Å)	<i>Sulfobolus Solfataricus</i> Thermophilic bact.	unknown	368	(Yano et al. 2000)

Bond					
P450 CYP51 4-Phenylimidazole Bond	1e9x (2.1 Å)	<i>Mycobacterium Tuberculosis</i>	14 α -sterol demethylase	455	(Podust et al. 2001)

Table 1: the eight X-ray crystal structures of P450s available in 2002: six bacterial, one fungal (P450_{nor}), one mammalian (CYP2C5). The P450_{cam}, P450_{terp}, P450_{eryF}, P450_{nor} belong to class I P450s enzymes, whereas P450_{BM3} belongs to class II enzymes, like microsomal enzymes CYP2C5 and 3A4. P450_{BM3} structure is therefore *a priori* more relevant to rebuilding a structural model of CYP3A4, but since the CYP2C5 X-Ray structure has been released, it became obvious that the structural homology between the other bacterial enzymes and microsomal enzymes was better than expected from the poor homology of primary structure (< 20%).

Then, the relevance of using class I and class II structures together for rebuilding models of class II P450s was no more questionable. The structural model of human CYP3A4 described in the present work was rebuilt using the six first structures listed above, with no preference in the structural alignment. The two last bacterial structural sets CYP51 and CYP119 were not incorporated into the modeling process.

All the proposed models of CYP3A4 obtained by homology modeling are thus so far based on bacterial crystal structure templates: the first was proposed by Ferenczy and Morris and used the X-ray structure of bacterial P450_{cam} as unique template structure (Ferenczy and Morris 1989). Another model was built later by David F.V. Lewis, using also a unique template structure, the P450_{BM3} structure, which was supposed to be more relevant as a template since this P450 was the only one class II enzyme with known three-dimensional structure (Lewis et al. 1996). A third model, based on a multiple structure template, was built by Szklarz and Halpert, using the four first X-ray crystal structures available P450_{cam}, P450_{terp}, P450_{eryF}, and P450_{BM3}. This four-bacterial template approach strategy is closer to our rebuilding strategy, but was still missing some relevance in the absence of a mammalian template. In our hands, the incorporation of the mammalian 2C5 crystal structure into rebuilding steps of models of cytochrome P450 3A4 proved to be decisive. Inclusion of 2C5 crystal structure had indeed a profound effect on the

structural alignment with the five non-mammalian structures, resulting in a different topology of the active site and a marked divergence between the model and each individual template. The advantage of our multiple-template approach resides essentially in the availability of a final template that can be used to rebuild various
5 mammalian cytochromes P450.

More recently, two new bacterial P450 crystal structures emerged in the literature (also listed in table 1): CYP51 (PDB code 1e9x), from *Mycobacterium tuberculosis*, that catalyzes the oxidative removal of 14 α -methyl group from sterol precursors in
10 sterol biosynthesis in yeast and fungi (ergosterol), plants (phytosterol) and mammals (cholesterol), for its potential in the design of antifungal agents (Podust et al. 2001). And CYP119 (PDB code 1f4t), from the thermophilic archaeon *Sulfolobus solfataricus*, the first P450 identified in *Archaea*, for its interest in understanding the enhanced thermal stability of the structure, especially in the
15 region of the active site (Yano et al. 2000). Those two structures have been shown to exhibit the typical bacterial P450 fold, with some exceptions in the topology. They have not been included as structural templates in the modeling steps of the present model. The names of newly discovered P450s follow the now accepted nomenclature of David R. Nelson (Nelson 1999).

20

The protein databank (Brookhaven Protein Databank, <http://www.rcsb.org/pdb/>) currently indicates that there are 76 separate crystal structures available for the eight crystallized P450s, plus 7 crystal structures on hold (Sept 1st, 2002), the majority of which containing either bond substrates or inhibitors. Table 1 provides the relevant
25 information about the structural templates used for human CYP3A4 model rebuilding. The idea behind homology modeling is that proteins belonging to the same functional class and showing a strong sequence similarity, adopt a similar fold (review in (Hilbert et al. 1993)). Known analogous structures are then used to generate a template or parent structure for the unknown protein to be modeled. The
30 reliability of the various methods employed depend mostly on the number of experimental 3D structures that can be aligned. Knowing that for pairs of distantly related proteins (with residue identity of about 20%) the regions having the same fold will represent less than half of each molecule, the regions where the folds differ

will predominate, and the divergence of sequence must be compensated by a higher number of homologous proteins to align (Chothia and Lesk 1986). Below 50% of sequence identity, the deviation in structurally not conserved regions becomes significant, and loop regions are difficult to predict. It is generally accepted that below 20% of sequence identity, the prediction turns out to be hazardous, and fold assignment methods are best replaced by *ab initio* methods, that ideally attempt to predict the native structure only from the primary sequence of the protein to be modeled. But produced models so far had the correct fold for only a few small protein domains (Sanchez et al. 2000).

10

Model rebuilding

The strategy of model rebuilding in the case of the P450 family is strongly driven by the low degree of homology between bacterial and mammalian cytochrome P450s (table 2).

15

PDB code	Swiss-Prot entry name	CP34_HUMAN	CP51_MYCTU	CPXW_SULSO	CPC5_RABIT	CPXA_PSEPU	CPXL_PSESP	CPXB_BACME	CPXJ_SACER	NOR_FUSOX
n.s.	CP34_HUMAN									
1E9X	CP51_MYCTU (CYP51)	22.30%								
1F4T	CPXW_SULSO (CYP119)	19%	21%							
1DT6	CPC5_RABIT (CYP2C5)	24.80%	19.40%	18.5%						
3CPP	CPXA_PSEPU (P450 cam)	19.20%	18.8%	21.7%	20%					
1CPT	CPXL_PSESP (P450 terp)	20%	23.2%	26.1%	20.2%	24.6%				
2HPD-A	CPXB_BACME (P450 BM3)	25.50%	22.6%	22.6%	21%	20.3%	23.4%			
1OXA	CPXJ_SACER (P450 eryF)	21.40%	22.8%	28.4%	18.5%	22.9%	25.1%	19.1%		
1ROM	NOR_FUSOX (P450 nor)	20.4%	20.3%	25.4%	16.9%	25.9%	27.8%	17.3%	30%	

Table 2: Sequence identities between the various crystallized cytochrome P450s and human CYP3A4 (source LALIGN, algorithm of Huang and Miller, published in Adv. Appl. Math. (1991) 12:337-357). For P450 BM3, Swissprot code name

CPXB_BACME, it corresponds to the fusion of P450 and a Reductase, thus is displays twice the number of residues; see <http://www.expasy.org/cgi-bin/niceprot.pl?P14779>

- 5 Our global scheme, which steps are described hereafter, is founded on a combination of methods developed in the literature for different purposes in protein structure determination studies. The principle of the primary steps, until the generation of a correct alignment of P450 primary sequences, is described in (Jean et al. 1997). The last steps are summarized in (Loiseau 2002).

10

Identification of common structural blocks (CSBs) between all selected 3D structures.

- CSBs define the common local folds which set up the vertebral column of the model (results in (Loiseau 2002)). The non conserved regions, that can be parts of
 15 secondary structures or non-structured regions as loops, will be rebuilt with no initial structural information.

Multiple alignment of crystalline P450s, on the basis of CSBs determination: the target sequence of human cytochrome P450 3A is aligned against the multiple
 20 alignment obtained from the CSBs of step 1 (with assessment of accuracy using online tools of multiple alignment such as CLUSTALW 1.8, etc..). This produces the key sequence alignment which allows the generation of the template structure used for the rebuilding of the various CYP3A models.

- 1) Generation of distance and dihedral angles constraints.
- 25 2) Selection of rotamers for side chains in CSBs.
- 3) Calculation of a set of structures using DYANA software. Loops are rebuilt between CSBs.
- 4) Structure optimization under XPLOR software.

30

Description

- Therefore, in a first aspect, the invention relates to a method for designing a 3-dimensional (3-D) model of a protein, the 3-dimensional representation of at least
5 three family members has already been experimentally obtained, [said 3-dimensional representation presenting similarities], comprising the steps of:
- a. identification of common structural blocks (CSB) among said members of said family,
 - b. alignment of the amino-acids primary sequence of said family members
10 according to said structural similarities, represented by said CSBs, in order to obtain a first alignment,
 - c. alignment of said protein as compared on said first alignment, in order to obtain a second alignment, wherein:
 - i. alignment of said protein is performed in order to maximize
15 the amino-acids alignment between said protein and said first alignment,
 - when one or more consensus amino-acid exists in said aligned structural blocs in said first alignment, and in the amino-acid
20 sequence of said protein, said consensus amino-acids are anchors of said second alignment,
 - ii. no insertion or deletion of amino-acids can be performed in the aligned CSBs, wherein insertion or deletions are possible
25 in non-aligned structural blocks, if better to align the primary amino-acids sequences,
 - d. definition of the atomic 3-D structure of structural blocs of said protein, according to the 3-D structure of the blocks of said family members,
 - e. definition of the local constraints (distance and angles) for the atoms that are not
30 structurally determined after step d. (that are not in the conserved structural blocks),
 - f. selection of rotamers,

- g. determination of a family of whole 3-D model structures of said protein, taking into account said atomic 3-D structure of structural blocs obtained in step d., said local constraints defined in step e., and said rotamers defined in step f.,
- h. optimization of said family of 3-D models obtained in step g., by
- 5 i. discarding sequences that present topological defects, and
- ii. recalculating 3-D structures by taking electrostatic forces into account, and performing the method again from step c. downward, with modifications in the alignment between the primary sequence of said protein and said first alignment, when the obtained model structures do not take
- 10 known efficient mutations into account.

In preferred embodiment, said 3-dimentional representation of family members has been obtained by crystallography or NMR.

The alignment of said common structural blocks in steps b. and c. can be performed

15 by use of the GOK software as described in Jean et al., 1997.

In addition, step d. is preferably performed according to the following rules:

- i. at a given position, when residues are identical between all the template structures and the target sequence, the 3D coordinates of the reference
- 20 residues are purely assigned to the target residue,
- ii. When residues differ, only the coordinates of the backbone atoms are assigned ($C\alpha$), and sometimes $C\beta$ when they exist.

In the above depicted method, the definition of local constraints in step e. is

25 performed by analysis of the allowed regions in Ramachandran diagram.

Furthermore, distances and angles are preferably selected in step e. by the following rules:

- i. all distances for which the lower bondary was less than 8 Å.
- 30 ii. all the distances involving at least one side-chain atom, to preserve the spatial arrangement between CSBs

- iii. all the distances involving atoms of any active group such as an heme group, to fix as much as possible the neighborhood of said active group, such as an iron atom

Angular constraints are preferably selected in step e. by the following rule:

- 5 i. dihedral angles ϕ and ψ of all residues located in CSBs are defined as constraints, given by the average values of corresponding ϕ , ψ angles in said family members +/- the standard deviation

10 To practice the method of the invention, rotamers in step f. can be selected from the couples according to the tables of Dunbrack and Karplus and step g. can be performed with the DYANA software, as described in Güntert et al, 1997.

In addition, the optimization in step h. comprises the use of the X-Plor software, as described in A. T. Brunger, X-PLOR, version 3.1. A system for X-ray
15 crystallography and NMR, Yale University Press, New Haven, CT (1992) and A. T. Brunger, Molecular replacement with X-PLOR: PC-refinement and free R value. In: Proceedings of the Daresbury Study Weekend on Molecular Replacement, Daresbury, United Kingdom (1992), 49-61.

20 The method according to the invention is particularly applicable to a cytochrome P450, such as the cytochrome P450 3A4 (SEQ ID N° 1). In this regards, for performing the first alignment can be performed using cytochrome P450 family members are chosen from Nor, (SEQ ID N° 2), Ery F (SEQ ID N° 3), terp (SEQ ID N° 4), Cam (SEQ ID N° 5), BM3 (SEQ ID N° 6) and 2C5 (SEQ ID N° 7).

25

In a second embodiment, the invention is directed to a model 3-D structure of a protein, obtained by the method as described above and more particularly to the cytochrome P450 3A4 model.

30 Regarding the P450 3A4 model, the main residues involved in the recognition of the substrate are C97; R104; F101; F107; F247; F303 and C376.

More specifically, R104 allows allows to capture the substrate that is near of the entry site and to accompany to the active site. F303 is implicated in the

recognition of the substrate in the active site. F107; F247 and F303 are involved in the recognition at the modulation site responsible for positive regulation.

For more details on F103 see : Domanski, T.L., et al., Analysis of four residues within substrate recognition site 4 of human cytochrome P450 3A4: role in
 5 steroid hydroxylase activity and alpha-naphthoflavone stimulation. Arch Biochem Biophys, 1998. 350(2): p. 223-32. (mutants I300, F303, A304, and T308).

10 Features of this model comprise the three dimensional atomic coordinates of Table 3, for C- α , and the (ϕ , ψ) couples of Table 4.

In a third embodiment, the invention contemplates a method for designing a protein, biological functions of which are altered, comprising:

- 15 a) obtaining a 3-D model of said protein by the method of as depicted above,
 b) analyzing said model of step a., and determining the amino-acids that are putatively involved in the biological functions of said protein,
 c) changing said amino-acids by mutating the corresponding nucleotides on the nucleic acid sequence coding for said protein, in order to obtain a mutated
 20 protein having altered properties.

In another embodiment, the invention relates to a computer-assisted method for performing restrained dynamics docking of a substrate on an enzyme, a 3-D structure of which is available, comprising the steps of

- 25 j. determining a force field, and independently simulating the presence of said enzyme in said force field,
 k. minimizing the potential energy (E_p) linked to said force field of said 3-D structure, wherein the spatial position some atoms of said enzyme is fixed, and wherein the other atoms are mobile, by allowing mobility of the mobile atoms,
 30 by
 i. simulating an increase in temperature (in order to give kinetic energy), and
 ii. minimizing the potential energy by re-specifying the temperature as 0 Kelvin (K);

- l. optionally repeating step b in order to obtain other E_p minima, wherein said E_p minima are such that the structure of the protein remains folded,
- m. minimizing E_p in said force field of said 3-D structure, wherein all the atoms of the protein are mobile, by
 - 5 i. simulating an increase in temperature (in order to give kinetic energy), and
 - ii. minimizing the potential energy by re-specifying the temperature as 0 Kelvin (K),
- n. simulating, at 0 K the presence of said substrate next to said enzyme,
- o. optionally generating a dynamic on said substrate and enzyme (simulating an
 - 10 increase in temperature, in order to allow mobility of the atoms),
- p. generating some constraints to said substrate, in order to impose that it has interaction with said enzyme,
- q. generating a dynamic on said substrate and enzyme, with said constraints imposed in step p.,
- 15 r. optionally, generating a dynamic on said substrate and enzyme without said constraints of step p.

In this method for performing restrained dynamics docking, said fixed atoms in step b. are the backbone atoms N-C α -CO in the first minimization step and only

20 C α in subsequent minimization steps.

In addition, kinetic energy is simulated by temperature increase to about 100 K for about 5-20 ns.

The force field in step a. comprises forces linked to

- a. the distance between atoms,
- 25 b. the angles of valence,
- c. the diedric angles,
- d. the deformation with regard to plan,
- e. the electrostatic field,
- f. the Van der Waals forces,
- 30 g. hydrogen bonds.

The constraints in step p. are attraction constraints to force said substrate in the active site, and wherein said constraints are not prejudiced to the exact spatial conformation of the substrate in the active site. These constraints are final

distance constraints between some atoms of said substrate and some atoms of amino-acids present in said active site.

Preferably, step o. is performed with a simulated temperature of between about
 5 15 and 50 K, step q. is performed with a simulated temperature of between about
 15 and 50 K, and step r. is performed with a simulated temperature of between
 about 200 and 350 K.

This method is particularly suited for multispecific protein such as a cytochrome
 10 P450. The cytochrome can be cytochrome P450 3A4, and said structure can be
 the structure obtained by the method of the invention described above, in
 particular the model structure defined with the features of Table 3 and 4.

The substrate can be a small organic compound which size can range for
 15 example from MW 288 (testosterone) to MW 1203 (cyclosporine A).

In a still another embodiment, the invention is aimed at a computer-assisted
 method for performing restrained dynamics docking of at least two substrates on
 an enzyme, a 3-D structure of which is available, consisting of performing the
 20 steps j, k, l, m, n, o, p, q and r depicted above with a first substrate and
 repeating said steps with a second substrate when the first substrate reaches an
 unconstrained molecular dynamic.

The first and second substrates can be the same molecule or different molecules.
 The first and second substrates can display either an allosteric or effect
 25 synergistic effect.

This method can be practiced with substrates that are inhibitors (competitive,
 uncompetitive, non competitive) or display an inhibitor-base mechanism. It can
 also be practice with an agonist and any molecule interfering with the biological
 30 function of the protein.

This method also embraces a successive repeat of the steps j, k, l, m, n, o, p, q and r depicted above with a 3rd, 4th or 5th substrate, some of them being the same or different molecules.

5 In this method for performing restrained dynamics docking, said fixed atoms in step b. are the backbone atoms N-C α -CO in the first minimization step and only C α in subsequent minimization steps.

In addition, kinetic energy is simulated by temperature increase to about 100 K for about 5-20 ns.

10 The force field in step a. comprises forces linked to

- a. the distance between atoms,
- b. the angles of valence,
- c. the diedric angles,
- d. the deformation with regard to plan,
- 15 e. the electrostatic field,
- f. the Van der Waals forces,
- g. hydrogen bonds.

The constraints in step p. are attraction constraints to force said substrate in the active site, and wherein said constraints are not prejudiced to the exact spatial
20 conformation of the substrate in the active site. These constraints are final distance constraints between some atoms of said substrate and some atoms of amino-acids present in said active site.

Preferably, step o. is performed with a simulated temperature of between about
25 15 and 50 K, step q. is performed with a simulated temperature of between about 15 and 50 K, and step r. is performed with a simulated temperature of between about 200 and 350 K.

This method is particularly suited for multispecific protein such as a cytochrome
30 P450. The cytochrome can be cytochrome P450 3A4, and said structure can be the structure obtained by the method of the invention described above, in particular the model structure defined with the features of Table 3 and 4.

TABLE 3

5	assign (segid 3A4 and resid 100 and name C) (segid 3A4 and resid 100 and name CB)	2.48	0.03	0.03
	assign (segid 3A4 and resid 100 and name C) (segid 3A4 and resid 100 and name O)	1.24	0.02	0.01
	assign (segid 3A4 and resid 100 and name C) (segid 3A4 and resid 101 and name C)	3.02	0.04	0.05
	assign (segid 3A4 and resid 100 and name C) (segid 3A4 and resid 101 and name CA)	2.43	0.02	0.02
	assign (segid 3A4 and resid 100 and name C) (segid 3A4 and resid 101 and name CB)	3.71	0.02	0.03
10	assign (segid 3A4 and resid 100 and name C) (segid 3A4 and resid 101 and name CG)	4.93	0.04	0.04
	assign (segid 3A4 and resid 100 and name C) (segid 3A4 and resid 101 and name N)	1.33	0.00	0.01
	assign (segid 3A4 and resid 100 and name C) (segid 3A4 and resid 101 and name O)	3.86	0.06	0.07
	assign (segid 3A4 and resid 100 and name C) (segid 3A4 and resid 102 and name C)	4.56	0.09	0.09
	assign (segid 3A4 and resid 100 and name C) (segid 3A4 and resid 102 and name CA)	4.47	0.08	0.08
15	assign (segid 3A4 and resid 100 and name C) (segid 3A4 and resid 102 and name N)	3.28	0.06	0.07
	assign (segid 3A4 and resid 100 and name C) (segid 3A4 and resid 102 and name O)	5.63	0.09	0.09
	assign (segid 3A4 and resid 100 and name C) (segid 3A4 and resid 103 and name C)	4.92	0.11	0.12
	assign (segid 3A4 and resid 100 and name C) (segid 3A4 and resid 103 and name CA)	4.58	0.13	0.13
	assign (segid 3A4 and resid 100 and name C) (segid 3A4 and resid 103 and name CB)	4.38	0.14	0.14
20	assign (segid 3A4 and resid 100 and name C) (segid 3A4 and resid 103 and name N)	3.82	0.12	0.13
	assign (segid 3A4 and resid 100 and name C) (segid 3A4 and resid 103 and name O)	6.14	0.12	0.11
	assign (segid 3A4 and resid 100 and name C) (segid 3A4 and resid 104 and name C)	6.18	0.12	0.13
	assign (segid 3A4 and resid 100 and name C) (segid 3A4 and resid 104 and name CA)	5.12	0.14	0.14
	assign (segid 3A4 and resid 100 and name C) (segid 3A4 and resid 104 and name CB)	4.72	0.17	0.18
25	assign (segid 3A4 and resid 100 and name C) (segid 3A4 and resid 104 and name N)	4.21	0.13	0.12
	assign (segid 3A4 and resid 100 and name C) (segid 3A4 and resid 104 and name O)	7.35	0.12	0.12
	assign (segid 3A4 and resid 100 and name C) (segid 3A4 and resid 105 and name CA)	7.32	0.16	0.16
	assign (segid 3A4 and resid 100 and name C) (segid 3A4 and resid 105 and name CB)	7.32	0.20	0.19
	assign (segid 3A4 and resid 100 and name C) (segid 3A4 and resid 105 and name N)	6.05	0.15	0.15
30	assign (segid 3A4 and resid 100 and name C) (segid 3A4 and resid 105 and name O)	1.51	0.01	0.01
	assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 100 and name C)	1.53	0.02	0.01
	assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 100 and name CB)	2.38	0.01	0.02
	assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 101 and name C)	4.41	0.04	0.04
	assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 101 and name CA)	3.81	0.02	0.01
35	assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 101 and name CB)	4.87	0.01	0.01
	assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 101 and name CG)	6.23	0.02	0.02
	assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 101 and name N)	2.45	0.02	0.01
	assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 101 and name O)	5.32	0.06	0.06
	assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 102 and name C)	5.52	0.11	0.11
40	assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 102 and name CA)	5.46	0.09	0.09
	assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 102 and name N)	4.38	0.07	0.07
	assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 102 and name O)	6.65	0.11	0.12
	assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 103 and name C)	5.80	0.18	0.18
	assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 103 and name CA)	5.21	0.18	0.18
45	assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 103 and name CB)	4.60	0.22	0.21
	assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 103 and name N)	4.60	0.14	0.14
	assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 103 and name O)	6.99	0.19	0.18
	assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 104 and name C)	7.45	0.16	0.17
	assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 104 and name CA)	6.28	0.19	0.19
50	assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 104 and name CB)	5.97	0.23	0.22
	assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 104 and name N)	5.27	0.17	0.18
	assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 105 and name CA)	8.70	0.16	0.16
	assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 105 and name CB)	8.72	0.19	0.18
	assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 105 and name N)	7.41	0.16	0.16
55	assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 106 and name CA)	10.03	0.14	0.13
	assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 106 and name CB)	9.61	0.16	0.17
	assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 107 and name CA)	10.68	0.13	0.13
	assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 107 and name CB)	9.93	0.14	0.14
	assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 108 and name CA)	12.45	0.16	0.16
60	assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 108 and name CB)	12.05	0.20	0.21
	assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 109 and name CA)	14.46	0.20	0.19
	assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 109 and name CB)	14.15	0.25	0.24
	assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 110 and name CA)	15.36	0.15	0.16
	assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 110 and name CB)	14.59	0.18	0.18
65	assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 111 and name CA)	17.01	0.47	0.48
	assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 111 and name CB)	16.41	0.61	0.62
	assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 112 and name CA)	19.32	0.20	0.20
	assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 123 and name CA)	18.93	0.57	0.57
70	assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 124 and name CA)	16.15	1.00	1.00
	assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 124 and name CB)	16.44	1.28	1.28
	assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 125 and name CA)	14.25	0.57	0.57
	assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 125 and name CB)	14.63	0.86	0.85
	assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 126 and name CA)	15.30	0.28	0.29
75	assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 127 and name CA)	15.07	1.25	1.26
	assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 127 and name CB)	15.82	1.74	1.73

assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 128 and name CA) 12.16 1.31 1.32
 assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 128 and name CB) 11.96 1.25 1.25
 assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 129 and name CA) 10.92 0.48 0.49
 assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 129 and name CB) 11.31 1.03 1.03
 assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 130 and name CA) 12.58 0.39 0.39
 5 assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 130 and name CB) 13.74 0.30 0.30
 assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 131 and name CA) 12.48 1.54 1.54
 assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 131 and name CB) 12.80 2.21 2.21
 assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 132 and name CA) 10.15 1.02 1.01
 assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 132 and name CB) 9.56 0.64 0.64
 10 assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 133 and name CA) 10.55 1.14 1.15
 assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 133 and name CB) 10.84 1.61 1.62
 assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 134 and name CA) 13.02 0.93 0.93
 assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 135 and name CA) 12.54 1.92 1.92
 assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 135 and name CB) 12.05 2.44 2.44
 15 assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 136 and name CA) 11.50 1.04 1.03
 assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 136 and name CB) 10.54 1.12 1.11
 assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 137 and name CA) 13.68 1.22 1.22
 assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 138 and name CA) 16.02 1.25 1.25
 assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 138 and name CB) 16.60 1.22 1.21
 20 assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 139 and name CA) 14.88 1.91 1.91
 assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 140 and name CA) 15.37 2.14 2.13
 assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 140 and name CB) 15.93 1.81 1.81
 assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 141 and name CA) 14.45 2.60 2.60
 assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 219 and name CA) 16.28 1.68 1.69
 25 assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 219 and name CB) 16.06 1.71 1.71
 assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 220 and name CB) 17.97 1.47 1.47
 assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 256 and name CA) 17.58 1.09 1.08
 assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 259 and name CA) 17.07 0.42 0.42
 assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 259 and name CB) 15.84 0.49 0.48
 30 assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 260 and name CA) 17.27 0.36 0.37
 assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 260 and name CB) 17.66 0.60 0.61
 assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 262 and name CB) 19.31 0.47 0.47
 assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 263 and name CA) 17.25 0.20 0.20
 assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 263 and name CB) 15.94 0.20 0.19
 35 assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 305 and name CB) 17.82 1.09 1.09
 assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 393 and name CA) 18.93 0.87 0.88
 assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 395 and name CA) 17.43 0.94 0.95
 assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 396 and name CA) 14.39 0.90 0.91
 assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 396 and name CB) 14.39 1.04 1.05
 40 assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 397 and name CA) 15.54 0.50 0.51
 assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 397 and name CB) 16.95 0.49 0.50
 assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 398 and name CA) 16.07 0.47 0.47
 assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 398 and name CB) 17.13 0.58 0.58
 assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 399 and name CA) 12.78 0.65 0.65
 45 assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 399 and name CB) 12.28 0.85 0.85
 assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 400 and name CA) 11.08 0.21 0.21
 assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 400 and name CB) 11.38 0.26 0.26
 assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 401 and name CA) 13.82 0.22 0.22
 50 assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 402 and name CA) 13.80 0.38 0.37
 assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 402 and name CB) 14.22 0.46 0.46
 assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 403 and name CA) 10.25 0.48 0.48
 assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 403 and name CB) 9.07 0.45 0.45
 assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 404 and name CA) 10.75 0.61 0.61
 55 assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 404 and name CB) 11.25 0.58 0.58
 assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 405 and name CA) 14.15 0.69 0.70
 assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 405 and name CB) 15.30 0.62 0.62
 assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 406 and name CA) 13.64 0.91 0.90
 assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 407 and name CA) 11.33 1.09 1.09
 60 assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 407 and name CB) 9.85 1.10 1.11
 assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 408 and name CA) 13.56 1.07 1.07
 assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 408 and name CB) 14.06 1.02 1.02
 assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 409 and name CA) 16.71 1.04 1.04
 assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 409 and name CB) 17.46 0.97 0.96
 assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 410 and name CA) 15.91 1.14 1.14
 65 assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 411 and name CA) 15.34 1.24 1.25
 assign (segid 3A4 and resid 100 and name CA) (segid 3A4 and resid 411 and name CB) 14.12 1.25 1.25
 assign (segid 3A4 and resid 100 and name CB) (segid 3A4 and resid 101 and name C) 5.39 0.04 0.05
 assign (segid 3A4 and resid 100 and name CB) (segid 3A4 and resid 101 and name CA) 4.43 0.06 0.07
 70 assign (segid 3A4 and resid 100 and name CB) (segid 3A4 and resid 101 and name CB) 5.29 0.10 0.10
 assign (segid 3A4 and resid 100 and name CB) (segid 3A4 and resid 101 and name CG) 6.64 0.12 0.11
 assign (segid 3A4 and resid 100 and name CB) (segid 3A4 and resid 101 and name N) 3.12 0.06 0.07
 assign (segid 3A4 and resid 100 and name CB) (segid 3A4 and resid 101 and name O) 6.27 0.05 0.04
 assign (segid 3A4 and resid 100 and name CB) (segid 3A4 and resid 102 and name C) 6.91 0.09 0.09
 assign (segid 3A4 and resid 100 and name CB) (segid 3A4 and resid 102 and name CA) 6.79 0.07 0.07
 75 assign (segid 3A4 and resid 100 and name CB) (segid 3A4 and resid 102 and name N) 5.58 0.06 0.07
 assign (segid 3A4 and resid 100 and name CB) (segid 3A4 and resid 103 and name C) 6.95 0.22 0.21
 assign (segid 3A4 and resid 100 and name CB) (segid 3A4 and resid 103 and name CA) 6.54 0.21 0.21
 assign (segid 3A4 and resid 100 and name CB) (segid 3A4 and resid 103 and name CB) 5.85 0.27 0.27
 80 assign (segid 3A4 and resid 100 and name CB) (segid 3A4 and resid 103 and name N) 6.02 0.15 0.14
 assign (segid 3A4 and resid 100 and name CB) (segid 3A4 and resid 104 and name CA) 7.04 0.24 0.24
 assign (segid 3A4 and resid 100 and name CB) (segid 3A4 and resid 104 and name CB) 6.45 0.28 0.29
 assign (segid 3A4 and resid 100 and name CB) (segid 3A4 and resid 104 and name N) 6.26 0.21 0.21

	assign (segid 3A4 and resid 100 and name CB)	(segid 3A4 and resid 105 and name CA)	9.69	0.20	0.19
	assign (segid 3A4 and resid 100 and name CB)	(segid 3A4 and resid 105 and name CB)	9.74	0.21	0.21
	assign (segid 3A4 and resid 100 and name CB)	(segid 3A4 and resid 106 and name CA)	11.28	0.17	0.17
	assign (segid 3A4 and resid 100 and name CB)	(segid 3A4 and resid 106 and name CB)	10.96	0.19	0.20
5	assign (segid 3A4 and resid 100 and name CB)	(segid 3A4 and resid 107 and name CA)	11.66	0.18	0.18
	assign (segid 3A4 and resid 100 and name CB)	(segid 3A4 and resid 107 and name CB)	10.79	0.20	0.21
	assign (segid 3A4 and resid 100 and name CB)	(segid 3A4 and resid 108 and name CA)	13.24	0.21	0.21
	assign (segid 3A4 and resid 100 and name CB)	(segid 3A4 and resid 108 and name CB)	12.77	0.27	0.26
	assign (segid 3A4 and resid 100 and name CB)	(segid 3A4 and resid 109 and name CA)	15.50	0.25	0.25
10	assign (segid 3A4 and resid 100 and name CB)	(segid 3A4 and resid 109 and name CB)	15.28	0.28	0.28
	assign (segid 3A4 and resid 100 and name CB)	(segid 3A4 and resid 110 and name CA)	16.45	0.21	0.20
	assign (segid 3A4 and resid 100 and name CB)	(segid 3A4 and resid 110 and name CB)	15.68	0.22	0.22
	assign (segid 3A4 and resid 100 and name CB)	(segid 3A4 and resid 111 and name CA)	17.86	0.53	0.54
	assign (segid 3A4 and resid 100 and name CB)	(segid 3A4 and resid 111 and name CB)	17.17	0.67	0.67
15	assign (segid 3A4 and resid 100 and name CB)	(segid 3A4 and resid 124 and name CA)	16.87	0.97	0.96
	assign (segid 3A4 and resid 100 and name CB)	(segid 3A4 and resid 124 and name CB)	17.23	1.24	1.25
	assign (segid 3A4 and resid 100 and name CB)	(segid 3A4 and resid 125 and name CA)	15.07	0.40	0.41
	assign (segid 3A4 and resid 100 and name CB)	(segid 3A4 and resid 125 and name CB)	15.55	0.69	0.68
	assign (segid 3A4 and resid 100 and name CB)	(segid 3A4 and resid 126 and name CA)	15.99	0.18	0.18
20	assign (segid 3A4 and resid 100 and name CB)	(segid 3A4 and resid 127 and name CA)	15.52	1.38	1.38
	assign (segid 3A4 and resid 100 and name CB)	(segid 3A4 and resid 127 and name CB)	16.25	1.81	1.82
	assign (segid 3A4 and resid 100 and name CB)	(segid 3A4 and resid 128 and name CA)	12.57	1.28	1.28
	assign (segid 3A4 and resid 100 and name CB)	(segid 3A4 and resid 128 and name CB)	12.46	1.13	1.13
	assign (segid 3A4 and resid 100 and name CB)	(segid 3A4 and resid 129 and name CA)	11.38	0.35	0.36
25	assign (segid 3A4 and resid 100 and name CB)	(segid 3A4 and resid 129 and name CB)	11.91	0.84	0.84
	assign (segid 3A4 and resid 100 and name CB)	(segid 3A4 and resid 130 and name CA)	12.76	0.56	0.56
	assign (segid 3A4 and resid 100 and name CB)	(segid 3A4 and resid 130 and name CB)	13.96	0.56	0.56
	assign (segid 3A4 and resid 100 and name CB)	(segid 3A4 and resid 131 and name CA)	12.39	1.79	1.78
	assign (segid 3A4 and resid 100 and name CB)	(segid 3A4 and resid 131 and name CB)	12.75	2.39	2.40
30	assign (segid 3A4 and resid 100 and name CB)	(segid 3A4 and resid 132 and name CA)	9.95	1.16	1.17
	assign (segid 3A4 and resid 100 and name CB)	(segid 3A4 and resid 132 and name CB)	9.49	0.72	0.73
	assign (segid 3A4 and resid 100 and name CB)	(segid 3A4 and resid 133 and name CA)	10.27	1.22	1.22
	assign (segid 3A4 and resid 100 and name CB)	(segid 3A4 and resid 133 and name CB)	10.70	1.58	1.58
	assign (segid 3A4 and resid 100 and name CB)	(segid 3A4 and resid 134 and name CA)	12.54	1.29	1.29
	assign (segid 3A4 and resid 100 and name CB)	(segid 3A4 and resid 135 and name CA)	11.82	2.22	2.22
35	assign (segid 3A4 and resid 100 and name CB)	(segid 3A4 and resid 135 and name CB)	11.36	2.72	2.72
	assign (segid 3A4 and resid 100 and name CB)	(segid 3A4 and resid 136 and name CA)	10.66	1.27	1.27
	assign (segid 3A4 and resid 100 and name CB)	(segid 3A4 and resid 136 and name CB)	9.77	1.33	1.33
	assign (segid 3A4 and resid 100 and name CB)	(segid 3A4 and resid 137 and name CA)	12.86	1.44	1.44
40	assign (segid 3A4 and resid 100 and name CB)	(segid 3A4 and resid 138 and name CA)	15.10	1.58	1.57
	assign (segid 3A4 and resid 100 and name CB)	(segid 3A4 and resid 138 and name CB)	15.73	1.55	1.55
	assign (segid 3A4 and resid 100 and name CB)	(segid 3A4 and resid 139 and name CA)	13.78	2.16	2.15
	assign (segid 3A4 and resid 100 and name CB)	(segid 3A4 and resid 140 and name CA)	14.37	2.36	2.36
	assign (segid 3A4 and resid 100 and name CB)	(segid 3A4 and resid 140 and name CB)	15.01	2.07	2.06
45	assign (segid 3A4 and resid 100 and name CB)	(segid 3A4 and resid 141 and name CA)	13.51	2.69	2.69
	assign (segid 3A4 and resid 100 and name CB)	(segid 3A4 and resid 141 and name CB)	13.96	3.50	3.51
	assign (segid 3A4 and resid 100 and name CB)	(segid 3A4 and resid 219 and name CA)	15.23	1.87	1.87
	assign (segid 3A4 and resid 100 and name CB)	(segid 3A4 and resid 219 and name CB)	14.98	1.90	1.89
	assign (segid 3A4 and resid 100 and name CB)	(segid 3A4 and resid 220 and name CA)	17.42	1.77	1.77
50	assign (segid 3A4 and resid 100 and name CB)	(segid 3A4 and resid 220 and name CB)	17.17	1.75	1.74
	assign (segid 3A4 and resid 100 and name CB)	(segid 3A4 and resid 256 and name CA)	17.71	1.39	1.39
	assign (segid 3A4 and resid 100 and name CB)	(segid 3A4 and resid 259 and name CA)	17.62	0.71	0.72
	assign (segid 3A4 and resid 100 and name CB)	(segid 3A4 and resid 259 and name CB)	16.33	0.78	0.79
	assign (segid 3A4 and resid 100 and name CB)	(segid 3A4 and resid 260 and name CA)	17.90	0.56	0.56
	assign (segid 3A4 and resid 100 and name CB)	(segid 3A4 and resid 260 and name CB)	18.21	0.75	0.75
55	assign (segid 3A4 and resid 100 and name CB)	(segid 3A4 and resid 263 and name CA)	18.24	0.28	0.27
	assign (segid 3A4 and resid 100 and name CB)	(segid 3A4 and resid 263 and name CB)	16.89	0.27	0.28
	assign (segid 3A4 and resid 100 and name CB)	(segid 3A4 and resid 395 and name CA)	17.71	1.13	1.12
	assign (segid 3A4 and resid 100 and name CB)	(segid 3A4 and resid 396 and name CA)	14.60	1.10	1.10
60	assign (segid 3A4 and resid 100 and name CB)	(segid 3A4 and resid 396 and name CB)	14.47	1.26	1.25
	assign (segid 3A4 and resid 100 and name CB)	(segid 3A4 and resid 397 and name CA)	16.00	0.74	0.74
	assign (segid 3A4 and resid 100 and name CB)	(segid 3A4 and resid 397 and name CB)	17.39	0.75	0.76
	assign (segid 3A4 and resid 100 and name CB)	(segid 3A4 and resid 398 and name CA)	16.74	0.62	0.63
	assign (segid 3A4 and resid 100 and name CB)	(segid 3A4 and resid 398 and name CB)	17.78	0.72	0.72
65	assign (segid 3A4 and resid 100 and name CB)	(segid 3A4 and resid 399 and name CA)	13.44	0.73	0.73
	assign (segid 3A4 and resid 100 and name CB)	(segid 3A4 and resid 399 and name CB)	12.81	0.93	0.93
	assign (segid 3A4 and resid 100 and name CB)	(segid 3A4 and resid 400 and name CA)	11.82	0.35	0.36
	assign (segid 3A4 and resid 100 and name CB)	(segid 3A4 and resid 400 and name CB)	12.01	0.44	0.44
	assign (segid 3A4 and resid 100 and name CB)	(segid 3A4 and resid 401 and name CA)	14.78	0.21	0.21
70	assign (segid 3A4 and resid 100 and name CB)	(segid 3A4 and resid 402 and name CA)	14.88	0.32	0.33
	assign (segid 3A4 and resid 100 and name CB)	(segid 3A4 and resid 402 and name CB)	15.24	0.45	0.46
	assign (segid 3A4 and resid 100 and name CB)	(segid 3A4 and resid 403 and name CA)	11.43	0.42	0.42
	assign (segid 3A4 and resid 100 and name CB)	(segid 3A4 and resid 403 and name CB)	10.17	0.39	0.40
	assign (segid 3A4 and resid 100 and name CB)	(segid 3A4 and resid 404 and name CA)	12.01	0.52	0.52
75	assign (segid 3A4 and resid 100 and name CB)	(segid 3A4 and resid 404 and name CB)	12.43	0.55	0.55
	assign (segid 3A4 and resid 100 and name CB)	(segid 3A4 and resid 405 and name CA)	15.47	0.58	0.57
	assign (segid 3A4 and resid 100 and name CB)	(segid 3A4 and resid 405 and name CB)	16.58	0.49	0.50
	assign (segid 3A4 and resid 100 and name CB)	(segid 3A4 and resid 406 and name CA)	15.00	0.85	0.85
	assign (segid 3A4 and resid 100 and name CB)	(segid 3A4 and resid 407 and name CA)	12.78	1.04	1.03
80	assign (segid 3A4 and resid 100 and name CB)	(segid 3A4 and resid 407 and name CB)	11.31	1.04	1.03
	assign (segid 3A4 and resid 100 and name CB)	(segid 3A4 and resid 408 and name CA)	14.98	0.97	0.96
	assign (segid 3A4 and resid 100 and name CB)	(segid 3A4 and resid 408 and name CB)	15.45	0.90	0.89
	assign (segid 3A4 and resid 100 and name CB)	(segid 3A4 and resid 410 and name CA)	17.34	1.13	1.14

	assign (segid 3A4 and resid 100 and name CB)	(segid 3A4 and resid 411 and name CA)	16.75	1.27	1.26
	assign (segid 3A4 and resid 100 and name CB)	(segid 3A4 and resid 411 and name CB)	15.51	1.25	1.25
	assign (segid 3A4 and resid 100 and name N)	(segid 3A4 and resid 100 and name C)	2.45	0.04	0.03
	assign (segid 3A4 and resid 100 and name N)	(segid 3A4 and resid 100 and name CA)	1.46	0.01	0.00
	assign (segid 3A4 and resid 100 and name N)	(segid 3A4 and resid 100 and name CB)	2.47	0.02	0.02
5	assign (segid 3A4 and resid 100 and name N)	(segid 3A4 and resid 100 and name O)	3.46	0.05	0.06
	assign (segid 3A4 and resid 100 and name N)	(segid 3A4 and resid 101 and name C)	4.71	0.05	0.05
	assign (segid 3A4 and resid 100 and name N)	(segid 3A4 and resid 101 and name CA)	4.25	0.04	0.03
	assign (segid 3A4 and resid 100 and name N)	(segid 3A4 and resid 101 and name CB)	5.04	0.07	0.08
	assign (segid 3A4 and resid 100 and name N)	(segid 3A4 and resid 101 and name CG)	6.49	0.07	0.07
10	assign (segid 3A4 and resid 100 and name N)	(segid 3A4 and resid 101 and name N)	2.86	0.03	0.03
	assign (segid 3A4 and resid 100 and name N)	(segid 3A4 and resid 101 and name O)	5.79	0.07	0.06
	assign (segid 3A4 and resid 100 and name N)	(segid 3A4 and resid 102 and name C)	5.62	0.08	0.07
	assign (segid 3A4 and resid 100 and name N)	(segid 3A4 and resid 102 and name CA)	5.30	0.09	0.08
	assign (segid 3A4 and resid 100 and name N)	(segid 3A4 and resid 102 and name N)	4.31	0.08	0.07
15	assign (segid 3A4 and resid 100 and name N)	(segid 3A4 and resid 102 and name O)	6.83	0.08	0.07
	assign (segid 3A4 and resid 100 and name N)	(segid 3A4 and resid 103 and name C)	6.51	0.13	0.14
	assign (segid 3A4 and resid 100 and name N)	(segid 3A4 and resid 103 and name CA)	5.65	0.14	0.14
	assign (segid 3A4 and resid 100 and name N)	(segid 3A4 and resid 103 and name CB)	5.12	0.21	0.20
	assign (segid 3A4 and resid 100 and name N)	(segid 3A4 and resid 103 and name N)	4.83	0.10	0.10
20	assign (segid 3A4 and resid 100 and name N)	(segid 3A4 and resid 104 and name CA)	7.31	0.13	0.13
	assign (segid 3A4 and resid 100 and name N)	(segid 3A4 and resid 104 and name CB)	7.10	0.16	0.16
	assign (segid 3A4 and resid 100 and name N)	(segid 3A4 and resid 104 and name N)	6.17	0.13	0.12
	assign (segid 3A4 and resid 100 and name N)	(segid 3A4 and resid 104 and name CB)	3.30	0.03	0.03
	assign (segid 3A4 and resid 100 and name O)	(segid 3A4 and resid 101 and name C)	2.97	0.07	0.06
25	assign (segid 3A4 and resid 100 and name O)	(segid 3A4 and resid 101 and name CA)	2.75	0.04	0.04
	assign (segid 3A4 and resid 100 and name O)	(segid 3A4 and resid 101 and name CB)	4.24	0.05	0.05
	assign (segid 3A4 and resid 100 and name O)	(segid 3A4 and resid 101 and name CG)	5.19	0.08	0.08
	assign (segid 3A4 and resid 100 and name O)	(segid 3A4 and resid 101 and name N)	2.24	0.02	0.02
	assign (segid 3A4 and resid 100 and name O)	(segid 3A4 and resid 101 and name O)	3.44	0.09	0.10
30	assign (segid 3A4 and resid 100 and name O)	(segid 3A4 and resid 102 and name C)	4.10	0.14	0.14
	assign (segid 3A4 and resid 100 and name O)	(segid 3A4 and resid 102 and name CA)	4.39	0.13	0.13
	assign (segid 3A4 and resid 100 and name O)	(segid 3A4 and resid 102 and name N)	3.43	0.08	0.09
	assign (segid 3A4 and resid 100 and name O)	(segid 3A4 and resid 102 and name O)	5.02	0.13	0.14
	assign (segid 3A4 and resid 100 and name O)	(segid 3A4 and resid 103 and name C)	3.87	0.13	0.12
35	assign (segid 3A4 and resid 100 and name O)	(segid 3A4 and resid 103 and name CA)	3.76	0.16	0.17
	assign (segid 3A4 and resid 100 and name O)	(segid 3A4 and resid 103 and name CB)	3.64	0.17	0.16
	assign (segid 3A4 and resid 100 and name O)	(segid 3A4 and resid 103 and name N)	3.28	0.18	0.18
	assign (segid 3A4 and resid 100 and name O)	(segid 3A4 and resid 103 and name O)	5.05	0.13	0.12
	assign (segid 3A4 and resid 100 and name O)	(segid 3A4 and resid 104 and name C)	5.10	0.16	0.17
40	assign (segid 3A4 and resid 100 and name O)	(segid 3A4 and resid 104 and name CA)	3.96	0.17	0.17
	assign (segid 3A4 and resid 100 and name O)	(segid 3A4 and resid 104 and name CB)	3.68	0.22	0.22
	assign (segid 3A4 and resid 100 and name O)	(segid 3A4 and resid 104 and name N)	3.06	0.15	0.14
	assign (segid 3A4 and resid 100 and name O)	(segid 3A4 and resid 104 and name O)	6.24	0.16	0.16
	assign (segid 3A4 and resid 100 and name O)	(segid 3A4 and resid 105 and name C)	7.34	0.17	0.16
45	assign (segid 3A4 and resid 100 and name O)	(segid 3A4 and resid 105 and name CA)	6.48	0.19	0.20
	assign (segid 3A4 and resid 100 and name O)	(segid 3A4 and resid 105 and name CB)	6.69	0.22	0.22
	assign (segid 3A4 and resid 100 and name O)	(segid 3A4 and resid 105 and name N)	5.13	0.19	0.20
	assign (segid 3A4 and resid 100 and name O)	(segid 3A4 and resid 106 and name N)	6.98	0.17	0.17
	assign (segid 3A4 and resid 100 and name O)	(segid 3A4 and resid 107 and name N)	7.83	0.08	0.09
50	assign (segid 3A4 and resid 101 and name C)	(segid 3A4 and resid 101 and name CB)	2.51	0.03	0.04
	assign (segid 3A4 and resid 101 and name C)	(segid 3A4 and resid 101 and name CG)	3.03	0.09	0.09
	assign (segid 3A4 and resid 101 and name C)	(segid 3A4 and resid 102 and name C)	1.23	0.01	0.00
	assign (segid 3A4 and resid 101 and name C)	(segid 3A4 and resid 102 and name CA)	2.43	0.01	0.01
55	assign (segid 3A4 and resid 101 and name C)	(segid 3A4 and resid 102 and name N)	1.32	0.01	0.01
	assign (segid 3A4 and resid 101 and name C)	(segid 3A4 and resid 102 and name O)	3.81	0.08	0.08
	assign (segid 3A4 and resid 101 and name C)	(segid 3A4 and resid 103 and name C)	4.51	0.11	0.12
	assign (segid 3A4 and resid 101 and name C)	(segid 3A4 and resid 103 and name CA)	4.43	0.06	0.07
	assign (segid 3A4 and resid 101 and name C)	(segid 3A4 and resid 103 and name CB)	5.19	0.06	0.06
60	assign (segid 3A4 and resid 101 and name C)	(segid 3A4 and resid 103 and name N)	3.25	0.07	0.06
	assign (segid 3A4 and resid 101 and name C)	(segid 3A4 and resid 103 and name O)	5.58	0.14	0.14
	assign (segid 3A4 and resid 101 and name C)	(segid 3A4 and resid 104 and name C)	4.86	0.12	0.11
	assign (segid 3A4 and resid 101 and name C)	(segid 3A4 and resid 104 and name CA)	4.53	0.11	0.11
65	assign (segid 3A4 and resid 101 and name C)	(segid 3A4 and resid 104 and name CB)	4.32	0.11	0.12
	assign (segid 3A4 and resid 101 and name C)	(segid 3A4 and resid 104 and name N)	3.81	0.10	0.10
	assign (segid 3A4 and resid 101 and name C)	(segid 3A4 and resid 104 and name O)	6.07	0.12	0.12
	assign (segid 3A4 and resid 101 and name C)	(segid 3A4 and resid 105 and name C)	6.12	0.12	0.12
	assign (segid 3A4 and resid 101 and name C)	(segid 3A4 and resid 105 and name CA)	5.05	0.15	0.14
70	assign (segid 3A4 and resid 101 and name C)	(segid 3A4 and resid 105 and name CB)	4.63	0.19	0.19
	assign (segid 3A4 and resid 101 and name C)	(segid 3A4 and resid 105 and name N)	4.14	0.12	0.12
	assign (segid 3A4 and resid 101 and name C)	(segid 3A4 and resid 105 and name O)	7.28	0.13	0.12
	assign (segid 3A4 and resid 101 and name C)	(segid 3A4 and resid 106 and name CA)	7.25	0.11	0.11
	assign (segid 3A4 and resid 101 and name C)	(segid 3A4 and resid 106 and name CB)	7.28	0.11	0.10
	assign (segid 3A4 and resid 101 and name C)	(segid 3A4 and resid 106 and name N)	5.97	0.11	0.12
75	assign (segid 3A4 and resid 101 and name C)	(segid 3A4 and resid 107 and name N)	7.78	0.12	0.12
	assign (segid 3A4 and resid 101 and name CA)	(segid 3A4 and resid 101 and name C)	1.52	0.01	0.01
	assign (segid 3A4 and resid 101 and name CA)	(segid 3A4 and resid 101 and name CB)	1.54	0.01	0.01
	assign (segid 3A4 and resid 101 and name CA)	(segid 3A4 and resid 101 and name CG)	2.53	0.02	0.03
	assign (segid 3A4 and resid 101 and name CA)	(segid 3A4 and resid 101 and name O)	2.39	0.02	0.02
80	assign (segid 3A4 and resid 101 and name CA)	(segid 3A4 and resid 102 and name C)	4.39	0.02	0.02
	assign (segid 3A4 and resid 101 and name CA)	(segid 3A4 and resid 102 and name CA)	3.81	0.01	0.00
	assign (segid 3A4 and resid 101 and name CA)	(segid 3A4 and resid 102 and name N)	2.43	0.02	0.01

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assign (segid 3A4 and resid 101 and name CA ) (segid 3A4 and resid 259 and name CA ) 14.12 0.59 0.59
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	assign (segid 3A4 and resid 101 and name CA) (segid 3A4 and resid 259 and name CB)	12.95	0.64	0.64
	assign (segid 3A4 and resid 101 and name CA) (segid 3A4 and resid 260 and name CA)	13.96	0.43	0.43
	assign (segid 3A4 and resid 101 and name CA) (segid 3A4 and resid 260 and name CB)	14.25	0.66	0.67
	assign (segid 3A4 and resid 101 and name CA) (segid 3A4 and resid 261 and name CA)	17.44	0.36	0.36
5	assign (segid 3A4 and resid 101 and name CA) (segid 3A4 and resid 262 and name CA)	16.94	0.63	0.63
	assign (segid 3A4 and resid 101 and name CA) (segid 3A4 and resid 262 and name CB)	16.54	0.81	0.82
	assign (segid 3A4 and resid 101 and name CA) (segid 3A4 and resid 263 and name CA)	14.39	0.41	0.41
	assign (segid 3A4 and resid 101 and name CA) (segid 3A4 and resid 263 and name CB)	12.99	0.37	0.38
	assign (segid 3A4 and resid 101 and name CA) (segid 3A4 and resid 264 and name CA)	16.83	0.33	0.34
10	assign (segid 3A4 and resid 101 and name CA) (segid 3A4 and resid 266 and name CA)	18.42	0.42	0.42
	assign (segid 3A4 and resid 101 and name CA) (segid 3A4 and resid 267 and name CA)	18.10	0.33	0.32
	assign (segid 3A4 and resid 101 and name CA) (segid 3A4 and resid 267 and name CB)	17.16	0.38	0.38
	assign (segid 3A4 and resid 101 and name CA) (segid 3A4 and resid 305 and name CB)	17.23	1.02	1.02
	assign (segid 3A4 and resid 101 and name CA) (segid 3A4 and resid 309 and name CA)	18.52	0.86	0.86
15	assign (segid 3A4 and resid 101 and name CA) (segid 3A4 and resid 309 and name CB)	17.40	0.94	0.93
	assign (segid 3A4 and resid 101 and name CA) (segid 3A4 and resid 393 and name CA)	17.31	1.04	1.04
	assign (segid 3A4 and resid 101 and name CA) (segid 3A4 and resid 394 and name CA)	18.16	1.13	1.13
	assign (segid 3A4 and resid 101 and name CA) (segid 3A4 and resid 395 and name CA)	16.50	1.36	1.37
	assign (segid 3A4 and resid 101 and name CA) (segid 3A4 and resid 396 and name CA)	13.16	1.28	1.27
20	assign (segid 3A4 and resid 101 and name CA) (segid 3A4 and resid 396 and name CB)	13.07	1.27	1.27
	assign (segid 3A4 and resid 101 and name CA) (segid 3A4 and resid 397 and name CA)	13.63	0.92	0.92
	assign (segid 3A4 and resid 101 and name CA) (segid 3A4 and resid 397 and name CB)	14.92	0.86	0.87
	assign (segid 3A4 and resid 101 and name CA) (segid 3A4 and resid 398 and name CA)	14.66	1.08	1.08
	assign (segid 3A4 and resid 101 and name CA) (segid 3A4 and resid 398 and name CB)	15.92	1.17	1.16
25	assign (segid 3A4 and resid 101 and name CA) (segid 3A4 and resid 399 and name CA)	11.88	1.32	1.32
	assign (segid 3A4 and resid 101 and name CA) (segid 3A4 and resid 399 and name CB)	11.61	1.48	1.48
	assign (segid 3A4 and resid 101 and name CA) (segid 3A4 and resid 400 and name CA)	9.32	0.87	0.87
	assign (segid 3A4 and resid 101 and name CA) (segid 3A4 and resid 400 and name CB)	9.31	0.78	0.77
	assign (segid 3A4 and resid 101 and name CA) (segid 3A4 and resid 401 and name CA)	11.90	0.62	0.63
30	assign (segid 3A4 and resid 101 and name CA) (segid 3A4 and resid 402 and name CA)	12.75	0.84	0.85
	assign (segid 3A4 and resid 101 and name CA) (segid 3A4 and resid 402 and name CB)	13.44	1.04	1.04
	assign (segid 3A4 and resid 101 and name CA) (segid 3A4 and resid 403 and name CA)	9.56	0.81	0.81
	assign (segid 3A4 and resid 101 and name CA) (segid 3A4 and resid 403 and name CB)	8.45	0.95	0.95
	assign (segid 3A4 and resid 101 and name CA) (segid 3A4 and resid 404 and name CA)	9.08	0.54	0.53
35	assign (segid 3A4 and resid 101 and name CA) (segid 3A4 and resid 404 and name CB)	9.15	0.66	0.65
	assign (segid 3A4 and resid 101 and name CA) (segid 3A4 and resid 405 and name CA)	12.71	0.52	0.52
	assign (segid 3A4 and resid 101 and name CA) (segid 3A4 and resid 405 and name CB)	13.81	0.54	0.55
	assign (segid 3A4 and resid 101 and name CA) (segid 3A4 and resid 406 and name CA)	13.15	0.50	0.50
	assign (segid 3A4 and resid 101 and name CA) (segid 3A4 and resid 407 and name CA)	10.94	0.46	0.46
40	assign (segid 3A4 and resid 101 and name CA) (segid 3A4 and resid 407 and name CB)	9.48	0.47	0.47
	assign (segid 3A4 and resid 101 and name CA) (segid 3A4 and resid 408 and name CA)	12.32	0.46	0.45
	assign (segid 3A4 and resid 101 and name CA) (segid 3A4 and resid 408 and name CB)	12.46	0.50	0.50
	assign (segid 3A4 and resid 101 and name CA) (segid 3A4 and resid 409 and name CA)	15.80	0.37	0.37
	assign (segid 3A4 and resid 101 and name CA) (segid 3A4 and resid 409 and name CB)	16.53	0.38	0.38
45	assign (segid 3A4 and resid 101 and name CA) (segid 3A4 and resid 410 and name CA)	15.77	0.50	0.50
	assign (segid 3A4 and resid 101 and name CA) (segid 3A4 and resid 411 and name CA)	14.97	0.64	0.64
	assign (segid 3A4 and resid 101 and name CA) (segid 3A4 and resid 411 and name CB)	13.66	0.69	0.68
	assign (segid 3A4 and resid 101 and name CA) (segid 3A4 and resid 412 and name CA)	17.15	0.84	0.84
50	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 101 and name CG)	1.52	0.01	0.01
	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 102 and name C)	5.43	0.02	0.01
	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 102 and name CA)	4.50	0.04	0.03
	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 102 and name N)	3.17	0.04	0.05
	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 102 and name O)	6.25	0.05	0.06
55	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 103 and name C)	6.87	0.12	0.12
	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 103 and name CA)	6.81	0.05	0.05
	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 103 and name CB)	7.30	0.06	0.07
	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 103 and name N)	5.62	0.06	0.05
	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 104 and name C)	6.79	0.18	0.19
60	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 104 and name CA)	6.41	0.18	0.17
	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 104 and name CB)	5.66	0.21	0.21
	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 104 and name N)	5.96	0.13	0.13
	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 105 and name CA)	6.91	0.20	0.20
	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 105 and name CB)	6.31	0.23	0.24
	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 105 and name N)	6.14	0.17	0.17
65	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 106 and name CA)	9.61	0.12	0.12
	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 106 and name CB)	9.73	0.09	0.09
	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 107 and name CA)	11.13	0.18	0.17
	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 107 and name CB)	10.80	0.20	0.21
	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 108 and name CA)	11.57	0.20	0.20
70	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 108 and name CB)	10.70	0.19	0.18
	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 109 and name CA)	13.22	0.32	0.32
	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 109 and name CB)	12.75	0.34	0.34
	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 110 and name CA)	15.26	0.19	0.19
	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 110 and name CB)	14.94	0.14	0.15
75	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 111 and name CA)	16.80	0.50	0.50
	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 111 and name CB)	16.24	0.69	0.68
	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 112 and name CA)	18.30	0.43	0.43
	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 121 and name CA)	15.77	0.67	0.67
	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 121 and name CB)	16.09	0.58	0.58
80	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 122 and name CA)	15.64	0.50	0.50
	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 122 and name CB)	16.93	0.44	0.45
	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 123 and name CA)	15.20	1.10	1.11
	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 123 and name CB)	16.35	1.31	1.31

	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 124 and name CA)	12.91	1.60	1.60
	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 124 and name CB)	13.50	1.83	1.82
	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 125 and name CA)	10.78	0.85	0.85
	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 125 and name CB)	11.38	0.73	0.73
5	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 126 and name CA)	11.28	0.52	0.53
	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 127 and name CA)	10.87	1.59	1.59
	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 127 and name CB)	11.73	2.00	1.99
	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 128 and name CA)	8.04	1.91	1.90
	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 128 and name CB)	8.11	1.92	1.91
10	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 129 and name C)	6.91	0.53	0.52
	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 129 and name CA)	6.75	0.66	0.66
	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 129 and name CB)	7.30	0.79	0.79
	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 129 and name O)	6.46	0.74	0.74
	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 130 and name CA)	8.29	0.17	0.16
15	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 130 and name CB)	9.45	0.15	0.14
	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 131 and name CA)	8.39	1.59	1.59
	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 131 and name CB)	8.74	2.29	2.29
	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 132 and name CA)	6.51	1.21	1.21
	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 132 and name CB)	5.95	1.16	1.15
20	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 133 and name CA)	7.11	1.00	1.01
	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 133 and name CB)	7.21	1.50	1.51
	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 133 and name N)	6.69	0.63	0.63
	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 134 and name CA)	9.71	0.31	0.31
	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 135 and name CA)	9.94	1.23	1.24
25	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 135 and name CB)	9.49	1.76	1.76
	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 136 and name CA)	9.64	0.60	0.61
	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 136 and name CB)	8.74	0.91	0.90
	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 137 and name CA)	11.61	0.75	0.75
	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 138 and name CA)	13.92	0.38	0.37
30	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 138 and name CB)	14.19	0.44	0.43
	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 139 and name CA)	13.51	1.20	1.19
	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 140 and name CA)	13.42	1.59	1.58
	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 140 and name CB)	13.67	1.24	1.25
	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 141 and name CA)	12.61	2.58	2.58
35	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 141 and name CB)	13.29	3.31	3.31
	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 147 and name CA)	14.67	2.72	2.73
	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 147 and name CB)	14.85	3.36	3.36
	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 149 and name CB)	15.86	1.93	1.94
	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 150 and name CA)	15.12	1.96	1.97
40	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 153 and name CB)	16.64	1.83	1.83
	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 219 and name CA)	15.42	0.81	0.82
	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 219 and name CB)	15.05	0.93	0.93
	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 220 and name CA)	16.68	0.64	0.64
	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 220 and name CB)	16.02	0.63	0.64
45	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 251 and name CA)	16.98	0.92	0.93
	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 251 and name CB)	16.65	1.05	1.04
	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 252 and name CA)	15.53	1.06	1.06
	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 252 and name CB)	16.07	1.25	1.26
50	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 253 and name CA)	17.73	0.73	0.73
	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 254 and name CA)	17.69	0.69	0.70
	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 255 and name CA)	14.32	0.99	0.99
	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 256 and name CA)	13.21	0.88	0.87
	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 257 and name CA)	15.89	0.72	0.72
55	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 258 and name CA)	16.34	0.54	0.55
	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 258 and name CB)	16.77	0.58	0.58
	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 259 and name CA)	13.04	0.59	0.58
	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 259 and name CB)	11.82	0.62	0.63
	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 260 and name CA)	13.06	0.53	0.53
	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 260 and name CB)	13.35	0.80	0.79
60	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 261 and name CA)	16.57	0.44	0.43
	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 262 and name CA)	16.10	0.72	0.71
	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 262 and name CB)	15.64	0.90	0.90
	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 263 and name CA)	13.79	0.51	0.51
	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 263 and name CB)	12.41	0.46	0.46
65	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 264 and name CA)	16.34	0.46	0.45
	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 265 and name CA)	19.18	0.51	0.50
	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 266 and name CA)	17.98	0.58	0.58
	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 267 and name CA)	17.91	0.43	0.42
	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 267 and name CB)	17.01	0.43	0.43
70	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 305 and name CB)	17.12	1.25	1.24
	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 309 and name CA)	17.93	1.08	1.09
	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 309 and name CB)	16.79	1.18	1.18
	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 393 and name CA)	16.00	1.07	1.06
	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 394 and name CA)	16.96	1.24	1.24
75	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 394 and name CB)	18.38	1.27	1.28
	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 395 and name CA)	15.42	1.53	1.52
	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 396 and name CA)	12.00	1.38	1.38
	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 396 and name CB)	11.85	1.31	1.30
	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 397 and name CA)	12.48	1.03	1.03
80	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 397 and name CB)	13.75	0.97	0.96
	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 398 and name CA)	13.73	1.30	1.30
	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 398 and name CB)	15.00	1.40	1.40
	assign (segid 3A4 and resid 101 and name CB) (segid 3A4 and resid 399 and name CA)	11.08	1.59	1.59

	assign (segid 3A4 and resid 101 and name CB)	(segid 3A4 and resid 399 and name CB)	10.77	1.74	1.73
	assign (segid 3A4 and resid 101 and name CB)	(segid 3A4 and resid 400 and name CA)	8.47	1.04	1.04
	assign (segid 3A4 and resid 101 and name CB)	(segid 3A4 and resid 400 and name CB)	8.31	0.88	0.88
	assign (segid 3A4 and resid 101 and name CB)	(segid 3A4 and resid 401 and name CA)	11.23	0.81	0.81
5	assign (segid 3A4 and resid 101 and name CB)	(segid 3A4 and resid 402 and name CA)	12.36	1.12	1.12
	assign (segid 3A4 and resid 101 and name CB)	(segid 3A4 and resid 402 and name CB)	13.02	1.33	1.32
	assign (segid 3A4 and resid 101 and name CB)	(segid 3A4 and resid 403 and name CA)	9.44	1.05	1.04
	assign (segid 3A4 and resid 101 and name CB)	(segid 3A4 and resid 403 and name CB)	8.27	1.18	1.17
	assign (segid 3A4 and resid 101 and name CB)	(segid 3A4 and resid 404 and name CA)	9.03	0.67	0.67
10	assign (segid 3A4 and resid 101 and name CB)	(segid 3A4 and resid 404 and name CB)	8.93	0.77	0.78
	assign (segid 3A4 and resid 101 and name CB)	(segid 3A4 and resid 405 and name CA)	12.70	0.68	0.69
	assign (segid 3A4 and resid 101 and name CB)	(segid 3A4 and resid 405 and name CB)	13.70	0.75	0.74
	assign (segid 3A4 and resid 101 and name CB)	(segid 3A4 and resid 406 and name CA)	13.40	0.69	0.69
	assign (segid 3A4 and resid 101 and name CB)	(segid 3A4 and resid 407 and name CA)	11.55	0.46	0.45
15	assign (segid 3A4 and resid 101 and name CB)	(segid 3A4 and resid 407 and name CB)	10.14	0.44	0.43
	assign (segid 3A4 and resid 101 and name CB)	(segid 3A4 and resid 408 and name CA)	12.84	0.35	0.36
	assign (segid 3A4 and resid 101 and name CB)	(segid 3A4 and resid 408 and name CB)	12.84	0.42	0.42
	assign (segid 3A4 and resid 101 and name CB)	(segid 3A4 and resid 409 and name CA)	16.29	0.35	0.36
	assign (segid 3A4 and resid 101 and name CB)	(segid 3A4 and resid 409 and name CB)	16.93	0.46	0.46
20	assign (segid 3A4 and resid 101 and name CB)	(segid 3A4 and resid 410 and name CA)	16.51	0.50	0.50
	assign (segid 3A4 and resid 101 and name CB)	(segid 3A4 and resid 411 and name CA)	15.89	0.52	0.51
	assign (segid 3A4 and resid 101 and name CB)	(segid 3A4 and resid 411 and name CB)	14.61	0.56	0.55
	assign (segid 3A4 and resid 101 and name CG)	(segid 3A4 and resid 412 and name CA)	17.90	0.72	0.72
25	assign (segid 3A4 and resid 101 and name CG)	(segid 3A4 and resid 102 and name C)	5.84	0.10	0.09
	assign (segid 3A4 and resid 101 and name CG)	(segid 3A4 and resid 102 and name CA)	4.93	0.16	0.16
	assign (segid 3A4 and resid 101 and name CG)	(segid 3A4 and resid 102 and name N)	3.88	0.15	0.14
	assign (segid 3A4 and resid 101 and name CG)	(segid 3A4 and resid 102 and name O)	6.42	0.13	0.13
	assign (segid 3A4 and resid 101 and name CG)	(segid 3A4 and resid 103 and name C)	7.23	0.14	0.14
30	assign (segid 3A4 and resid 101 and name CG)	(segid 3A4 and resid 103 and name CA)	7.40	0.06	0.05
	assign (segid 3A4 and resid 101 and name CG)	(segid 3A4 and resid 103 and name N)	6.26	0.06	0.05
	assign (segid 3A4 and resid 101 and name CG)	(segid 3A4 and resid 104 and name C)	6.55	0.24	0.25
	assign (segid 3A4 and resid 101 and name CG)	(segid 3A4 and resid 104 and name CA)	6.45	0.26	0.26
	assign (segid 3A4 and resid 101 and name CG)	(segid 3A4 and resid 104 and name CB)	5.65	0.34	0.35
	assign (segid 3A4 and resid 101 and name CG)	(segid 3A4 and resid 104 and name N)	6.27	0.17	0.17
35	assign (segid 3A4 and resid 101 and name CG)	(segid 3A4 and resid 104 and name O)	7.59	0.29	0.29
	assign (segid 3A4 and resid 101 and name CG)	(segid 3A4 and resid 105 and name C)	7.71	0.15	0.15
	assign (segid 3A4 and resid 101 and name CG)	(segid 3A4 and resid 105 and name CA)	6.33	0.18	0.18
	assign (segid 3A4 and resid 101 and name CG)	(segid 3A4 and resid 105 and name CB)	5.64	0.23	0.23
	assign (segid 3A4 and resid 101 and name CG)	(segid 3A4 and resid 105 and name N)	5.80	0.17	0.17
40	assign (segid 3A4 and resid 101 and name CG)	(segid 3A4 and resid 129 and name C)	5.90	0.62	0.63
	assign (segid 3A4 and resid 101 and name CG)	(segid 3A4 and resid 129 and name CA)	5.70	0.77	0.78
	assign (segid 3A4 and resid 101 and name CG)	(segid 3A4 and resid 129 and name CB)	6.33	0.86	0.86
	assign (segid 3A4 and resid 101 and name CG)	(segid 3A4 and resid 129 and name O)	5.59	0.91	0.91
	assign (segid 3A4 and resid 101 and name CG)	(segid 3A4 and resid 130 and name CA)	7.31	0.19	0.19
45	assign (segid 3A4 and resid 101 and name CG)	(segid 3A4 and resid 130 and name N)	6.73	0.30	0.29
	assign (segid 3A4 and resid 101 and name CG)	(segid 3A4 and resid 133 and name N)	6.25	0.88	0.88
	assign (segid 3A4 and resid 101 and name N)	(segid 3A4 and resid 101 and name C)	2.44	0.03	0.03
	assign (segid 3A4 and resid 101 and name N)	(segid 3A4 and resid 101 and name CA)	1.45	0.01	0.01
	assign (segid 3A4 and resid 101 and name N)	(segid 3A4 and resid 101 and name CB)	2.46	0.01	0.01
50	assign (segid 3A4 and resid 101 and name N)	(segid 3A4 and resid 101 and name CG)	3.80	0.01	0.01
	assign (segid 3A4 and resid 101 and name N)	(segid 3A4 and resid 101 and name O)	3.48	0.03	0.03
	assign (segid 3A4 and resid 101 and name N)	(segid 3A4 and resid 102 and name C)	4.68	0.04	0.04
	assign (segid 3A4 and resid 101 and name N)	(segid 3A4 and resid 102 and name CA)	4.19	0.05	0.04
	assign (segid 3A4 and resid 101 and name N)	(segid 3A4 and resid 102 and name N)	2.78	0.05	0.05
55	assign (segid 3A4 and resid 101 and name N)	(segid 3A4 and resid 102 and name O)	5.75	0.05	0.06
	assign (segid 3A4 and resid 101 and name N)	(segid 3A4 and resid 103 and name C)	5.63	0.07	0.07
	assign (segid 3A4 and resid 101 and name N)	(segid 3A4 and resid 103 and name CA)	5.33	0.07	0.07
	assign (segid 3A4 and resid 101 and name N)	(segid 3A4 and resid 103 and name CB)	5.40	0.10	0.10
	assign (segid 3A4 and resid 101 and name N)	(segid 3A4 and resid 103 and name N)	4.30	0.07	0.07
60	assign (segid 3A4 and resid 101 and name N)	(segid 3A4 and resid 103 and name O)	6.84	0.07	0.07
	assign (segid 3A4 and resid 101 and name N)	(segid 3A4 and resid 104 and name C)	6.47	0.06	0.07
	assign (segid 3A4 and resid 101 and name N)	(segid 3A4 and resid 104 and name CA)	5.64	0.07	0.06
	assign (segid 3A4 and resid 101 and name N)	(segid 3A4 and resid 104 and name CB)	5.09	0.10	0.09
	assign (segid 3A4 and resid 101 and name N)	(segid 3A4 and resid 104 and name N)	4.84	0.06	0.06
65	assign (segid 3A4 and resid 101 and name N)	(segid 3A4 and resid 104 and name O)	7.67	0.06	0.07
	assign (segid 3A4 and resid 101 and name N)	(segid 3A4 and resid 105 and name CA)	7.25	0.13	0.12
	assign (segid 3A4 and resid 101 and name N)	(segid 3A4 and resid 105 and name CB)	7.00	0.18	0.19
	assign (segid 3A4 and resid 101 and name N)	(segid 3A4 and resid 105 and name N)	6.12	0.10	0.11
	assign (segid 3A4 and resid 101 and name N)	(segid 3A4 and resid 105 and name CB)	3.28	0.05	0.06
70	assign (segid 3A4 and resid 101 and name O)	(segid 3A4 and resid 101 and name CG)	3.29	0.09	0.08
	assign (segid 3A4 and resid 101 and name O)	(segid 3A4 and resid 102 and name C)	2.93	0.04	0.04
	assign (segid 3A4 and resid 101 and name O)	(segid 3A4 and resid 102 and name CA)	2.76	0.03	0.02
	assign (segid 3A4 and resid 101 and name O)	(segid 3A4 and resid 102 and name N)	2.23	0.01	0.02
	assign (segid 3A4 and resid 101 and name O)	(segid 3A4 and resid 102 and name O)	3.38	0.08	0.08
75	assign (segid 3A4 and resid 101 and name O)	(segid 3A4 and resid 103 and name C)	4.05	0.17	0.18
	assign (segid 3A4 and resid 101 and name O)	(segid 3A4 and resid 103 and name CA)	4.33	0.12	0.12
	assign (segid 3A4 and resid 101 and name O)	(segid 3A4 and resid 103 and name CB)	5.31	0.13	0.13
	assign (segid 3A4 and resid 101 and name O)	(segid 3A4 and resid 103 and name N)	3.38	0.11	0.10
	assign (segid 3A4 and resid 101 and name O)	(segid 3A4 and resid 103 and name O)	4.96	0.21	0.21
80	assign (segid 3A4 and resid 101 and name O)	(segid 3A4 and resid 104 and name C)	3.81	0.16	0.15
	assign (segid 3A4 and resid 101 and name O)	(segid 3A4 and resid 104 and name CA)	3.74	0.16	0.17
	assign (segid 3A4 and resid 101 and name O)	(segid 3A4 and resid 104 and name CB)	3.63	0.16	0.17
	assign (segid 3A4 and resid 101 and name O)	(segid 3A4 and resid 104 and name N)	3.29	0.16	0.16

	assign (segid 3A4 and resid 101 and name O) (segid 3A4 and resid 104 and name O)	4.99	0.16	0.15
	assign (segid 3A4 and resid 101 and name O) (segid 3A4 and resid 105 and name C)	5.02	0.13	0.13
	assign (segid 3A4 and resid 101 and name O) (segid 3A4 and resid 105 and name CB)	3.87	0.15	0.14
	assign (segid 3A4 and resid 101 and name O) (segid 3A4 and resid 105 and name CB)	3.56	0.21	0.22
5	assign (segid 3A4 and resid 101 and name O) (segid 3A4 and resid 105 and name N)	2.99	0.13	0.14
	assign (segid 3A4 and resid 101 and name O) (segid 3A4 and resid 105 and name O)	6.14	0.13	0.14
	assign (segid 3A4 and resid 101 and name O) (segid 3A4 and resid 106 and name C)	7.22	0.12	0.12
	assign (segid 3A4 and resid 101 and name O) (segid 3A4 and resid 106 and name CB)	6.38	0.13	0.13
	assign (segid 3A4 and resid 101 and name O) (segid 3A4 and resid 106 and name CB)	6.62	0.11	0.11
10	assign (segid 3A4 and resid 101 and name O) (segid 3A4 and resid 106 and name N)	5.02	0.13	0.13
	assign (segid 3A4 and resid 101 and name O) (segid 3A4 and resid 107 and name CB)	7.79	0.19	0.20
	assign (segid 3A4 and resid 101 and name O) (segid 3A4 and resid 107 and name N)	6.87	0.15	0.14
	assign (segid 3A4 and resid 102 and name C) (segid 3A4 and resid 102 and name O)	1.23	0.00	0.01
	assign (segid 3A4 and resid 102 and name C) (segid 3A4 and resid 103 and name C)	3.05	0.06	0.05
15	assign (segid 3A4 and resid 102 and name C) (segid 3A4 and resid 103 and name CA)	2.44	0.02	0.02
	assign (segid 3A4 and resid 102 and name C) (segid 3A4 and resid 103 and name CB)	3.70	0.03	0.04
	assign (segid 3A4 and resid 102 and name C) (segid 3A4 and resid 103 and name N)	1.32	0.01	0.02
	assign (segid 3A4 and resid 102 and name C) (segid 3A4 and resid 103 and name O)	3.88	0.10	0.09
	assign (segid 3A4 and resid 102 and name C) (segid 3A4 and resid 104 and name C)	4.57	0.06	0.07
20	assign (segid 3A4 and resid 102 and name C) (segid 3A4 and resid 104 and name CA)	4.51	0.04	0.04
	assign (segid 3A4 and resid 102 and name C) (segid 3A4 and resid 104 and name CB)	5.25	0.05	0.04
	assign (segid 3A4 and resid 102 and name C) (segid 3A4 and resid 104 and name N)	3.34	0.03	0.04
	assign (segid 3A4 and resid 102 and name C) (segid 3A4 and resid 104 and name O)	5.64	0.09	0.08
	assign (segid 3A4 and resid 102 and name C) (segid 3A4 and resid 105 and name C)	4.89	0.09	0.09
25	assign (segid 3A4 and resid 102 and name C) (segid 3A4 and resid 105 and name CA)	4.56	0.08	0.07
	assign (segid 3A4 and resid 102 and name C) (segid 3A4 and resid 105 and name CB)	4.34	0.12	0.12
	assign (segid 3A4 and resid 102 and name C) (segid 3A4 and resid 105 and name N)	3.84	0.08	0.07
	assign (segid 3A4 and resid 102 and name C) (segid 3A4 and resid 105 and name O)	6.11	0.10	0.09
	assign (segid 3A4 and resid 102 and name C) (segid 3A4 and resid 106 and name C)	6.12	0.09	0.09
30	assign (segid 3A4 and resid 102 and name C) (segid 3A4 and resid 106 and name CA)	5.05	0.08	0.09
	assign (segid 3A4 and resid 102 and name C) (segid 3A4 and resid 106 and name CB)	4.64	0.08	0.09
	assign (segid 3A4 and resid 102 and name C) (segid 3A4 and resid 106 and name N)	4.15	0.09	0.09
	assign (segid 3A4 and resid 102 and name C) (segid 3A4 and resid 106 and name O)	7.29	0.09	0.09
	assign (segid 3A4 and resid 102 and name C) (segid 3A4 and resid 107 and name CA)	7.22	0.12	0.11
35	assign (segid 3A4 and resid 102 and name C) (segid 3A4 and resid 107 and name CB)	7.24	0.11	0.11
	assign (segid 3A4 and resid 102 and name C) (segid 3A4 and resid 107 and name N)	5.94	0.11	0.12
	assign (segid 3A4 and resid 102 and name C) (segid 3A4 and resid 403 and name C)	7.21	0.28	0.28
	assign (segid 3A4 and resid 102 and name C) (segid 3A4 and resid 403 and name O)	6.84	0.38	0.38
	assign (segid 3A4 and resid 102 and name C) (segid 3A4 and resid 407 and name CB)	5.86	0.70	0.70
40	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 102 and name C)	1.53	0.01	0.01
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 103 and name C)	2.39	0.00	0.01
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 103 and name CA)	4.44	0.06	0.07
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 103 and name CB)	3.83	0.02	0.02
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 103 and name N)	4.87	0.05	0.04
45	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 103 and name O)	2.45	0.03	0.02
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 104 and name C)	5.34	0.09	0.10
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 104 and name CA)	5.54	0.09	0.08
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 104 and name CB)	5.50	0.05	0.06
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 104 and name N)	5.91	0.07	0.07
50	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 104 and name O)	4.45	0.04	0.04
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 105 and name C)	6.66	0.10	0.09
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 105 and name CA)	5.75	0.11	0.10
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 105 and name CB)	5.17	0.11	0.11
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 105 and name N)	4.53	0.14	0.14
55	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 105 and name O)	4.60	0.11	0.11
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 106 and name C)	6.93	0.12	0.12
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 106 and name CB)	7.39	0.09	0.08
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 106 and name N)	6.20	0.09	0.09
60	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 106 and name O)	5.87	0.11	0.11
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 107 and name CB)	5.22	0.09	0.09
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 107 and name N)	8.62	0.10	0.09
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 107 and name O)	8.66	0.09	0.09
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 108 and name CA)	7.31	0.10	0.11
65	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 108 and name CB)	10.01	0.09	0.10
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 109 and name CA)	9.60	0.16	0.16
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 109 and name CB)	10.76	0.17	0.17
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 110 and name CA)	10.03	0.23	0.22
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 110 and name CB)	12.29	0.10	0.10
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 111 and name CA)	11.86	0.13	0.13
70	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 111 and name CB)	14.62	0.31	0.31
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 112 and name CA)	14.39	0.48	0.47
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 112 and name CB)	16.16	0.20	0.20
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 119 and name CB)	15.93	1.64	1.64
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 121 and name CA)	14.19	1.16	1.16
75	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 121 and name CB)	14.24	1.08	1.09
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 122 and name CA)	15.01	1.12	1.12
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 122 and name CB)	16.43	1.12	1.12
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 123 and name CA)	15.15	1.20	1.20
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 123 and name CB)	16.30	1.27	1.28
80	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 124 and name CA)	12.35	1.42	1.41
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 124 and name CB)	12.51	1.63	1.64
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 125 and name CA)	9.99	1.22	1.22
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 125 and name CB)	10.09	1.37	1.37

	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 126 and name CA)	11.30	1.18	1.18
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 127 and name CA)	11.91	1.28	1.27
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 127 and name CB)	12.69	1.68	1.69
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 128 and name CA)	9.38	1.69	1.69
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 128 and name CB)	8.94	1.89	1.89
5	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 129 and name CA)	8.07	1.27	1.28
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 129 and name CB)	7.91	1.78	1.77
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 130 and name CA)	10.57	1.06	1.06
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 130 and name CB)	11.49	1.04	1.04
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 131 and name CA)	11.43	1.07	1.07
10	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 131 and name CB)	11.63	1.66	1.65
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 132 and name CA)	9.88	0.86	0.86
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 132 and name CB)	9.00	0.84	0.83
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 133 and name CA)	10.65	1.18	1.19
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 133 and name CB)	10.46	1.77	1.77
15	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 134 and name CA)	13.42	0.33	0.32
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 135 and name CA)	13.81	0.99	1.00
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 135 and name CB)	13.27	1.48	1.47
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 136 and name CA)	13.48	0.52	0.52
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 136 and name CB)	12.45	0.72	0.73
20	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 137 and name CA)	15.48	0.83	0.83
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 138 and name CA)	17.92	0.30	0.31
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 138 and name CB)	18.19	0.35	0.34
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 139 and name CA)	17.55	1.13	1.12
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 140 and name CA)	17.44	1.36	1.37
25	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 140 and name CB)	17.65	1.01	1.01
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 141 and name CA)	16.50	2.24	2.23
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 255 and name CA)	16.64	0.61	0.61
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 256 and name CA)	15.38	0.57	0.57
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 257 and name CA)	17.37	0.69	0.68
30	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 258 and name CA)	17.35	0.51	0.52
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 258 and name CB)	17.93	0.50	0.50
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 259 and name CA)	13.70	0.49	0.49
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 259 and name CB)	12.75	0.44	0.43
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 260 and name CA)	13.41	0.91	0.91
35	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 260 and name CB)	13.98	1.08	1.08
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 261 and name CA)	16.52	0.77	0.78
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 262 and name CA)	15.54	0.45	0.44
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 262 and name CB)	15.22	0.29	0.30
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 263 and name CA)	12.55	0.64	0.64
40	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 263 and name CB)	11.27	0.71	0.70
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 264 and name CA)	15.04	0.82	0.82
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 265 and name CA)	17.78	0.75	0.76
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 266 and name CA)	15.99	0.65	0.65
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 267 and name CA)	15.44	0.78	0.77
45	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 267 and name CB)	14.58	0.90	0.90
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 270 and name CB)	17.38	0.75	0.75
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 280 and name CA)	17.79	0.35	0.36
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 280 and name CB)	16.93	0.44	0.43
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 281 and name CA)	17.24	0.35	0.34
50	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 281 and name CB)	17.68	0.46	0.45
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 305 and name CA)	15.62	0.72	0.71
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 305 and name CB)	14.30	0.76	0.76
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 306 and name CA)	16.59	0.63	0.62
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 308 and name CA)	18.24	0.64	0.64
55	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 308 and name CB)	17.38	0.69	0.69
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 309 and name CA)	16.23	0.52	0.53
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 309 and name CB)	15.22	0.49	0.48
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 312 and name CB)	17.86	0.82	0.82
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 393 and name CA)	17.94	0.26	0.27
60	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 394 and name CA)	18.06	0.28	0.28
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 394 and name CB)	19.37	0.32	0.32
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 395 and name CA)	16.39	0.56	0.57
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 396 and name CA)	13.48	0.44	0.44
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 396 and name CB)	13.76	0.47	0.46
65	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 397 and name CA)	13.33	0.14	0.14
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 397 and name CB)	14.61	0.20	0.19
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 398 and name CA)	13.59	0.26	0.26
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 398 and name CB)	14.82	0.36	0.36
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 399 and name CA)	10.94	0.58	0.59
70	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 399 and name CB)	11.07	0.76	0.76
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 400 and name CA)	8.41	0.20	0.19
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 400 and name CB)	8.81	0.34	0.34
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 401 and name CA)	10.05	0.48	0.49
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 402 and name CA)	10.41	0.28	0.29
75	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 402 and name CB)	11.27	0.46	0.47
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 403 and name C)	6.42	0.29	0.29
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 403 and name CA)	7.08	0.37	0.36
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 403 and name CB)	6.38	0.51	0.50
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 403 and name O)	6.29	0.35	0.34
80	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 404 and name CA)	6.17	0.74	0.74
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 404 and name CB)	6.58	0.86	0.86
	assign (segid 3A4 and resid 102 and name CA) (segid 3A4 and resid 404 and name N)	6.38	0.44	0.44

	assign (segid 3A4 and resid 102 and name CA)	(segid 3A4 and resid 405 and name CA)	9.61	0.70	0.70
	assign (segid 3A4 and resid 102 and name CA)	(segid 3A4 and resid 405 and name CB)	10.83	0.65	0.66
	assign (segid 3A4 and resid 102 and name CA)	(segid 3A4 and resid 406 and name CA)	9.89	0.41	0.41
	assign (segid 3A4 and resid 102 and name CA)	(segid 3A4 and resid 407 and name CA)	7.52	0.53	0.53
5	assign (segid 3A4 and resid 102 and name CA)	(segid 3A4 and resid 407 and name CB)	6.11	0.56	0.56
	assign (segid 3A4 and resid 102 and name CA)	(segid 3A4 and resid 408 and name CA)	8.94	0.91	0.90
	assign (segid 3A4 and resid 102 and name CA)	(segid 3A4 and resid 408 and name CB)	9.18	1.03	1.02
	assign (segid 3A4 and resid 102 and name CA)	(segid 3A4 and resid 409 and name CA)	12.32	0.68	0.69
	assign (segid 3A4 and resid 102 and name CA)	(segid 3A4 and resid 409 and name CB)	13.07	0.67	0.66
10	assign (segid 3A4 and resid 102 and name CA)	(segid 3A4 and resid 410 and name CA)	12.35	0.55	0.56
	assign (segid 3A4 and resid 102 and name CA)	(segid 3A4 and resid 411 and name CA)	11.76	0.67	0.66
	assign (segid 3A4 and resid 102 and name CA)	(segid 3A4 and resid 411 and name CB)	10.53	0.73	0.74
	assign (segid 3A4 and resid 102 and name CA)	(segid 3A4 and resid 412 and name CA)	13.92	1.01	1.01
	assign (segid 3A4 and resid 102 and name CA)	(segid 3A4 and resid 414 and name CA)	17.92	1.15	1.15
15	assign (segid 3A4 and resid 102 and name N)	(segid 3A4 and resid 102 and name C)	2.45	0.02	0.02
	assign (segid 3A4 and resid 102 and name N)	(segid 3A4 and resid 102 and name CA)	1.46	0.01	0.01
	assign (segid 3A4 and resid 102 and name N)	(segid 3A4 and resid 102 and name O)	3.48	0.04	0.03
	assign (segid 3A4 and resid 102 and name N)	(segid 3A4 and resid 103 and name C)	4.70	0.08	0.09
	assign (segid 3A4 and resid 102 and name N)	(segid 3A4 and resid 103 and name CA)	4.21	0.04	0.04
20	assign (segid 3A4 and resid 102 and name N)	(segid 3A4 and resid 103 and name CB)	4.96	0.06	0.07
	assign (segid 3A4 and resid 102 and name N)	(segid 3A4 and resid 103 and name N)	2.80	0.04	0.04
	assign (segid 3A4 and resid 102 and name N)	(segid 3A4 and resid 103 and name O)	5.79	0.11	0.10
	assign (segid 3A4 and resid 102 and name N)	(segid 3A4 and resid 104 and name C)	5.63	0.07	0.08
	assign (segid 3A4 and resid 102 and name N)	(segid 3A4 and resid 104 and name CA)	5.33	0.07	0.08
25	assign (segid 3A4 and resid 102 and name N)	(segid 3A4 and resid 104 and name CB)	5.38	0.07	0.08
	assign (segid 3A4 and resid 102 and name N)	(segid 3A4 and resid 104 and name N)	4.34	0.06	0.06
	assign (segid 3A4 and resid 102 and name N)	(segid 3A4 and resid 104 and name O)	6.84	0.08	0.07
	assign (segid 3A4 and resid 102 and name N)	(segid 3A4 and resid 105 and name C)	6.48	0.09	0.09
	assign (segid 3A4 and resid 102 and name N)	(segid 3A4 and resid 105 and name CA)	5.63	0.11	0.11
30	assign (segid 3A4 and resid 102 and name N)	(segid 3A4 and resid 105 and name CB)	5.07	0.15	0.14
	assign (segid 3A4 and resid 102 and name N)	(segid 3A4 and resid 105 and name N)	4.83	0.09	0.10
	assign (segid 3A4 and resid 102 and name N)	(segid 3A4 and resid 105 and name O)	7.67	0.09	0.10
	assign (segid 3A4 and resid 102 and name N)	(segid 3A4 and resid 106 and name CA)	7.24	0.08	0.09
35	assign (segid 3A4 and resid 102 and name N)	(segid 3A4 and resid 106 and name CB)	7.02	0.09	0.10
	assign (segid 3A4 and resid 102 and name N)	(segid 3A4 and resid 106 and name N)	6.11	0.08	0.08
	assign (segid 3A4 and resid 102 and name N)	(segid 3A4 and resid 106 and name O)	7.23	0.34	0.34
	assign (segid 3A4 and resid 102 and name N)	(segid 3A4 and resid 403 and name CB)	6.74	0.63	0.63
	assign (segid 3A4 and resid 102 and name N)	(segid 3A4 and resid 404 and name N)	7.17	0.38	0.39
40	assign (segid 3A4 and resid 102 and name O)	(segid 3A4 and resid 103 and name C)	3.02	0.04	0.03
	assign (segid 3A4 and resid 102 and name O)	(segid 3A4 and resid 103 and name CA)	2.78	0.04	0.04
	assign (segid 3A4 and resid 102 and name O)	(segid 3A4 and resid 103 and name CB)	4.25	0.04	0.05
	assign (segid 3A4 and resid 102 and name O)	(segid 3A4 and resid 103 and name N)	2.25	0.02	0.02
	assign (segid 3A4 and resid 102 and name O)	(segid 3A4 and resid 103 and name O)	3.48	0.08	0.09
45	assign (segid 3A4 and resid 102 and name O)	(segid 3A4 and resid 104 and name C)	4.15	0.11	0.10
	assign (segid 3A4 and resid 102 and name O)	(segid 3A4 and resid 104 and name CA)	4.44	0.08	0.09
	assign (segid 3A4 and resid 102 and name O)	(segid 3A4 and resid 104 and name CB)	5.40	0.11	0.10
	assign (segid 3A4 and resid 102 and name O)	(segid 3A4 and resid 104 and name N)	3.51	0.08	0.08
	assign (segid 3A4 and resid 102 and name O)	(segid 3A4 and resid 104 and name O)	5.05	0.13	0.14
50	assign (segid 3A4 and resid 102 and name O)	(segid 3A4 and resid 105 and name C)	3.84	0.11	0.12
	assign (segid 3A4 and resid 102 and name O)	(segid 3A4 and resid 105 and name CA)	3.77	0.09	0.09
	assign (segid 3A4 and resid 102 and name O)	(segid 3A4 and resid 105 and name CB)	3.64	0.12	0.11
	assign (segid 3A4 and resid 102 and name O)	(segid 3A4 and resid 105 and name N)	3.32	0.08	0.09
	assign (segid 3A4 and resid 102 and name O)	(segid 3A4 and resid 105 and name O)	5.02	0.12	0.12
55	assign (segid 3A4 and resid 102 and name O)	(segid 3A4 and resid 106 and name C)	5.03	0.09	0.10
	assign (segid 3A4 and resid 102 and name O)	(segid 3A4 and resid 106 and name CA)	3.88	0.09	0.08
	assign (segid 3A4 and resid 102 and name O)	(segid 3A4 and resid 106 and name CB)	3.57	0.06	0.06
	assign (segid 3A4 and resid 102 and name O)	(segid 3A4 and resid 106 and name N)	3.01	0.11	0.10
	assign (segid 3A4 and resid 102 and name O)	(segid 3A4 and resid 106 and name O)	6.17	0.09	0.09
60	assign (segid 3A4 and resid 102 and name O)	(segid 3A4 and resid 107 and name C)	7.27	0.12	0.11
	assign (segid 3A4 and resid 102 and name O)	(segid 3A4 and resid 107 and name CA)	6.38	0.11	0.11
	assign (segid 3A4 and resid 102 and name O)	(segid 3A4 and resid 107 and name CB)	6.62	0.10	0.10
	assign (segid 3A4 and resid 102 and name O)	(segid 3A4 and resid 107 and name N)	5.02	0.12	0.12
	assign (segid 3A4 and resid 102 and name O)	(segid 3A4 and resid 108 and name N)	6.98	0.16	0.16
65	assign (segid 3A4 and resid 102 and name O)	(segid 3A4 and resid 403 and name C)	7.46	0.26	0.25
	assign (segid 3A4 and resid 102 and name O)	(segid 3A4 and resid 403 and name O)	7.00	0.30	0.29
	assign (segid 3A4 and resid 102 and name O)	(segid 3A4 and resid 404 and name N)	7.43	0.35	0.36
	assign (segid 3A4 and resid 102 and name O)	(segid 3A4 and resid 407 and name CA)	7.00	0.55	0.54
	assign (segid 3A4 and resid 102 and name O)	(segid 3A4 and resid 407 and name CB)	5.68	0.52	0.52
70	assign (segid 3A4 and resid 103 and name C)	(segid 3A4 and resid 103 and name CB)	2.49	0.01	0.01
	assign (segid 3A4 and resid 103 and name C)	(segid 3A4 and resid 103 and name O)	1.23	0.01	0.01
	assign (segid 3A4 and resid 103 and name C)	(segid 3A4 and resid 104 and name C)	3.01	0.05	0.04
	assign (segid 3A4 and resid 103 and name C)	(segid 3A4 and resid 104 and name CA)	2.43	0.01	0.01
	assign (segid 3A4 and resid 103 and name C)	(segid 3A4 and resid 104 and name CB)	3.71	0.01	0.01
	assign (segid 3A4 and resid 103 and name C)	(segid 3A4 and resid 104 and name N)	1.32	0.00	0.01
75	assign (segid 3A4 and resid 103 and name C)	(segid 3A4 and resid 104 and name O)	3.84	0.10	0.09
	assign (segid 3A4 and resid 103 and name C)	(segid 3A4 and resid 105 and name C)	4.56	0.06	0.07
	assign (segid 3A4 and resid 103 and name C)	(segid 3A4 and resid 105 and name CA)	4.46	0.06	0.06
	assign (segid 3A4 and resid 103 and name C)	(segid 3A4 and resid 105 and name CB)	5.21	0.09	0.09
	assign (segid 3A4 and resid 103 and name C)	(segid 3A4 and resid 105 and name N)	3.28	0.06	0.06
80	assign (segid 3A4 and resid 103 and name C)	(segid 3A4 and resid 105 and name O)	5.64	0.09	0.08
	assign (segid 3A4 and resid 103 and name C)	(segid 3A4 and resid 106 and name C)	4.91	0.06	0.06
	assign (segid 3A4 and resid 103 and name C)	(segid 3A4 and resid 106 and name CA)	4.60	0.03	0.04
	assign (segid 3A4 and resid 103 and name C)	(segid 3A4 and resid 106 and name CB)	4.43	0.07	0.07

	assign (segid 3A4 and resid 103 and name C)	(segid 3A4 and resid 106 and name N)	3.84	0.05	0.05
	assign (segid 3A4 and resid 103 and name C)	(segid 3A4 and resid 106 and name O)	6.12	0.06	0.07
	assign (segid 3A4 and resid 103 and name C)	(segid 3A4 and resid 107 and name C)	6.08	0.12	0.11
	assign (segid 3A4 and resid 103 and name C)	(segid 3A4 and resid 107 and name CA)	4.99	0.10	0.09
	assign (segid 3A4 and resid 103 and name C)	(segid 3A4 and resid 107 and name CB)	4.56	0.08	0.09
5	assign (segid 3A4 and resid 103 and name C)	(segid 3A4 and resid 107 and name N)	4.12	0.09	0.08
	assign (segid 3A4 and resid 103 and name C)	(segid 3A4 and resid 107 and name O)	7.23	0.11	0.11
	assign (segid 3A4 and resid 103 and name C)	(segid 3A4 and resid 108 and name CA)	7.24	0.11	0.12
	assign (segid 3A4 and resid 103 and name C)	(segid 3A4 and resid 108 and name CB)	7.26	0.17	0.16
	assign (segid 3A4 and resid 103 and name C)	(segid 3A4 and resid 108 and name N)	5.97	0.10	0.10
10	assign (segid 3A4 and resid 103 and name C)	(segid 3A4 and resid 109 and name N)	7.84	0.09	0.10
	assign (segid 3A4 and resid 103 and name C)	(segid 3A4 and resid 103 and name C)	1.52	0.01	0.01
	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 103 and name CB)	1.52	0.02	0.01
	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 103 and name O)	2.39	0.02	0.03
	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 104 and name C)	4.39	0.05	0.05
15	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 104 and name CA)	3.80	0.01	0.02
	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 104 and name CB)	4.86	0.03	0.03
	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 104 and name N)	2.44	0.03	0.02
	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 104 and name O)	5.29	0.10	0.10
	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 105 and name C)	5.49	0.09	0.09
20	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 105 and name CA)	5.43	0.06	0.07
	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 105 and name CB)	5.85	0.10	0.11
	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 105 and name N)	4.36	0.06	0.06
	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 105 and name O)	6.62	0.10	0.10
	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 106 and name C)	5.72	0.11	0.11
25	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 106 and name CA)	5.16	0.08	0.08
	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 106 and name CB)	4.55	0.07	0.08
	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 106 and name N)	4.55	0.09	0.09
	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 106 and name O)	6.93	0.10	0.11
	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 107 and name C)	7.31	0.15	0.16
30	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 107 and name CA)	6.10	0.14	0.14
	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 107 and name CB)	5.77	0.13	0.13
	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 107 and name N)	5.13	0.13	0.13
	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 108 and name CA)	8.61	0.15	0.14
	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 108 and name CB)	8.65	0.18	0.18
35	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 108 and name N)	7.30	0.13	0.14
	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 109 and name CA)	9.96	0.09	0.09
	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 109 and name CB)	9.60	0.15	0.15
	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 109 and name N)	10.43	0.12	0.11
	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 110 and name CA)	9.62	0.15	0.15
40	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 111 and name CA)	12.59	0.36	0.36
	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 111 and name CB)	12.28	0.48	0.48
	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 112 and name CA)	14.87	0.18	0.18
	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 112 and name CB)	16.15	1.42	1.41
	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 119 and name CB)	15.59	0.89	0.88
45	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 121 and name CA)	15.73	0.89	0.90
	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 122 and name CA)	16.97	0.74	0.74
	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 122 and name CB)	18.46	0.74	0.73
	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 123 and name CA)	16.68	0.56	0.57
	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 123 and name CB)	17.65	0.72	0.72
50	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 124 and name CA)	13.43	0.81	0.81
	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 124 and name CB)	13.31	1.13	1.12
	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 125 and name CA)	11.84	0.88	0.89
	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 125 and name CB)	11.90	1.36	1.35
	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 126 and name CA)	13.78	0.88	0.89
55	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 127 and name CA)	14.13	0.93	0.93
	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 127 and name CB)	14.66	1.54	1.54
	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 128 and name CA)	11.58	1.05	1.04
	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 128 and name CB)	10.95	1.06	1.07
	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 129 and name CA)	10.90	1.08	1.08
60	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 129 and name CB)	10.88	1.71	1.72
	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 130 and name CA)	13.49	0.69	0.69
	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 130 and name CB)	14.39	0.51	0.51
	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 131 and name CA)	13.83	1.01	1.00
	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 131 and name CB)	13.82	1.68	1.68
65	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 132 and name CA)	12.13	0.68	0.68
	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 132 and name CB)	11.21	0.67	0.68
	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 133 and name CA)	13.26	1.46	1.46
	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 133 and name CB)	13.31	1.91	1.91
	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 134 and name CA)	15.88	0.68	0.69
70	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 135 and name CA)	15.76	1.30	1.30
	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 135 and name CB)	15.07	1.68	1.68
	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 136 and name CA)	15.35	1.07	1.07
	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 136 and name CB)	14.37	1.33	1.34
	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 137 and name CA)	17.68	1.26	1.25
75	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 137 and name CB)	17.14	0.15	0.14
	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 259 and name CA)	16.21	0.16	0.17
	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 259 and name CB)	16.51	0.44	0.44
	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 260 and name CA)	16.96	0.62	0.62
	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 260 and name CB)	18.75	0.26	0.26
80	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 262 and name CA)	18.55	0.16	0.16
	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 262 and name CB)	15.50	0.43	0.44
	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 263 and name CA)	14.24	0.42	0.41
	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 263 and name CB)			

	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 264 and name CA)	17.58	0.60	0.60
	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 267 and name CA)	17.46	0.88	0.88
	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 267 and name CB)	16.52	0.93	0.93
	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 305 and name CA)	17.69	1.07	1.07
5	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 305 and name CB)	16.29	1.11	1.10
	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 309 and name CB)	18.17	0.61	0.60
	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 396 and name CA)	16.79	0.63	0.62
	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 396 and name CB)	17.03	0.72	0.73
	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 397 and name CA)	16.86	0.18	0.19
	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 397 and name CB)	18.17	0.14	0.14
10	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 398 and name CA)	16.95	0.28	0.27
	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 398 and name CB)	18.12	0.35	0.34
	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 399 and name CA)	14.10	0.49	0.49
	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 399 and name CB)	14.15	0.68	0.67
	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 400 and name CA)	11.85	0.17	0.17
15	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 400 and name CB)	12.32	0.22	0.23
	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 401 and name CA)	13.35	0.49	0.48
	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 402 and name CA)	13.20	0.41	0.41
	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 402 and name CB)	14.02	0.38	0.39
	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 403 and name CA)	9.64	0.41	0.40
20	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 403 and name CB)	9.10	0.39	0.39
	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 404 and name CA)	8.83	0.72	0.71
	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 404 and name CB)	9.50	0.69	0.69
	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 405 and name CA)	11.68	0.96	0.95
	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 405 and name CB)	13.07	0.90	0.90
25	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 406 and name CA)	11.22	0.94	0.95
	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 407 and name CA)	7.97	1.17	1.17
	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 407 and name CB)	6.59	1.15	1.15
	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 408 and name CA)	9.46	1.38	1.39
	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 408 and name CB)	10.15	1.39	1.39
30	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 409 and name CA)	12.71	1.32	1.33
	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 409 and name CB)	13.74	1.27	1.26
	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 410 and name CA)	11.90	1.30	1.29
	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 411 and name CA)	10.61	1.40	1.40
	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 411 and name CB)	9.27	1.42	1.43
35	assign (segid 3A4 and resid 103 and name CA)	(segid 3A4 and resid 412 and name CA)	13.30	1.55	1.55
	assign (segid 3A4 and resid 103 and name CB)	(segid 3A4 and resid 104 and name C)	5.41	0.04	0.04
	assign (segid 3A4 and resid 103 and name CB)	(segid 3A4 and resid 104 and name CA)	4.47	0.04	0.04
	assign (segid 3A4 and resid 103 and name CB)	(segid 3A4 and resid 104 and name CB)	5.34	0.06	0.07
	assign (segid 3A4 and resid 103 and name CB)	(segid 3A4 and resid 104 and name N)	3.14	0.03	0.03
40	assign (segid 3A4 and resid 103 and name CB)	(segid 3A4 and resid 104 and name O)	6.27	0.09	0.08
	assign (segid 3A4 and resid 103 and name CB)	(segid 3A4 and resid 105 and name C)	6.90	0.08	0.08
	assign (segid 3A4 and resid 103 and name CB)	(segid 3A4 and resid 105 and name CA)	6.80	0.06	0.05
	assign (segid 3A4 and resid 103 and name CB)	(segid 3A4 and resid 105 and name CB)	7.28	0.10	0.09
	assign (segid 3A4 and resid 103 and name CB)	(segid 3A4 and resid 105 and name N)	5.60	0.05	0.06
45	assign (segid 3A4 and resid 103 and name CB)	(segid 3A4 and resid 106 and name C)	6.88	0.12	0.11
	assign (segid 3A4 and resid 103 and name CB)	(segid 3A4 and resid 106 and name CA)	6.50	0.08	0.08
	assign (segid 3A4 and resid 103 and name CB)	(segid 3A4 and resid 106 and name CB)	5.80	0.08	0.08
	assign (segid 3A4 and resid 103 and name CB)	(segid 3A4 and resid 106 and name N)	5.98	0.08	0.09
	assign (segid 3A4 and resid 103 and name CB)	(segid 3A4 and resid 107 and name CA)	6.88	0.15	0.14
50	assign (segid 3A4 and resid 103 and name CB)	(segid 3A4 and resid 107 and name CB)	6.27	0.15	0.15
	assign (segid 3A4 and resid 103 and name CB)	(segid 3A4 and resid 107 and name N)	6.13	0.13	0.13
	assign (segid 3A4 and resid 103 and name CB)	(segid 3A4 and resid 108 and name CA)	9.60	0.13	0.13
	assign (segid 3A4 and resid 103 and name CB)	(segid 3A4 and resid 108 and name CB)	9.70	0.17	0.16
	assign (segid 3A4 and resid 103 and name CB)	(segid 3A4 and resid 109 and name CA)	11.20	0.10	0.09
55	assign (segid 3A4 and resid 103 and name CB)	(segid 3A4 and resid 109 and name CB)	10.93	0.14	0.15
	assign (segid 3A4 and resid 103 and name CB)	(segid 3A4 and resid 110 and name CA)	11.35	0.14	0.13
	assign (segid 3A4 and resid 103 and name CB)	(segid 3A4 and resid 110 and name CB)	10.40	0.16	0.16
	assign (segid 3A4 and resid 103 and name CB)	(segid 3A4 and resid 111 and name CA)	13.37	0.37	0.37
	assign (segid 3A4 and resid 103 and name CB)	(segid 3A4 and resid 111 and name CB)	12.99	0.48	0.47
60	assign (segid 3A4 and resid 103 and name CB)	(segid 3A4 and resid 112 and name CA)	15.89	0.19	0.19
	assign (segid 3A4 and resid 103 and name CB)	(segid 3A4 and resid 121 and name CA)	17.03	0.82	0.82
	assign (segid 3A4 and resid 103 and name CB)	(segid 3A4 and resid 121 and name CB)	17.19	0.86	0.86
	assign (segid 3A4 and resid 103 and name CB)	(segid 3A4 and resid 122 and name CA)	18.38	0.65	0.64
	assign (segid 3A4 and resid 103 and name CB)	(segid 3A4 and resid 123 and name CA)	18.01	0.43	0.43
65	assign (segid 3A4 and resid 103 and name CB)	(segid 3A4 and resid 124 and name CA)	14.77	0.73	0.72
	assign (segid 3A4 and resid 103 and name CB)	(segid 3A4 and resid 124 and name CB)	14.66	1.06	1.05
	assign (segid 3A4 and resid 103 and name CB)	(segid 3A4 and resid 125 and name CA)	13.23	0.80	0.80
	assign (segid 3A4 and resid 103 and name CB)	(segid 3A4 and resid 125 and name CB)	13.32	1.30	1.29
	assign (segid 3A4 and resid 103 and name CB)	(segid 3A4 and resid 126 and name CA)	15.08	0.77	0.77
70	assign (segid 3A4 and resid 103 and name CB)	(segid 3A4 and resid 127 and name CA)	15.31	0.97	0.97
	assign (segid 3A4 and resid 103 and name CB)	(segid 3A4 and resid 127 and name CB)	15.84	1.58	1.59
	assign (segid 3A4 and resid 103 and name CB)	(segid 3A4 and resid 128 and name CA)	12.67	1.05	1.04
	assign (segid 3A4 and resid 103 and name CB)	(segid 3A4 and resid 128 and name CB)	12.10	1.01	1.01
	assign (segid 3A4 and resid 103 and name CB)	(segid 3A4 and resid 129 and name CA)	11.93	1.01	1.01
75	assign (segid 3A4 and resid 103 and name CB)	(segid 3A4 and resid 129 and name CB)	12.00	1.63	1.64
	assign (segid 3A4 and resid 103 and name CB)	(segid 3A4 and resid 130 and name CA)	14.35	0.67	0.66
	assign (segid 3A4 and resid 103 and name CB)	(segid 3A4 and resid 130 and name CB)	15.30	0.46	0.46
	assign (segid 3A4 and resid 103 and name CB)	(segid 3A4 and resid 131 and name CA)	14.54	1.19	1.20
	assign (segid 3A4 and resid 103 and name CB)	(segid 3A4 and resid 131 and name CB)	14.57	1.86	1.87
80	assign (segid 3A4 and resid 103 and name CB)	(segid 3A4 and resid 132 and name CA)	12.67	0.90	0.90
	assign (segid 3A4 and resid 103 and name CB)	(segid 3A4 and resid 132 and name CB)	11.81	0.85	0.85
	assign (segid 3A4 and resid 103 and name CB)	(segid 3A4 and resid 133 and name CA)	13.68	1.52	1.53

	assign (segid 3A4 and resid 103 and name CB)	(segid 3A4 and resid 133 and name CB)	13.80	1.94	1.95
	assign (segid 3A4 and resid 103 and name CB)	(segid 3A4 and resid 131 and name CA)	16.25	0.90	0.91
	assign (segid 3A4 and resid 103 and name CB)	(segid 3A4 and resid 135 and name CA)	15.96	1.61	1.61
	assign (segid 3A4 and resid 103 and name CB)	(segid 3A4 and resid 135 and name CB)	15.30	1.99	1.99
5	assign (segid 3A4 and resid 103 and name CB)	(segid 3A4 and resid 136 and name CA)	15.36	1.32	1.33
	assign (segid 3A4 and resid 103 and name CB)	(segid 3A4 and resid 136 and name CB)	14.38	1.54	1.55
	assign (segid 3A4 and resid 103 and name CB)	(segid 3A4 and resid 137 and name CA)	17.70	1.44	1.43
	assign (segid 3A4 and resid 103 and name CB)	(segid 3A4 and resid 259 and name CA)	18.19	0.15	0.15
	assign (segid 3A4 and resid 103 and name CB)	(segid 3A4 and resid 259 and name CB)	17.20	0.22	0.23
10	assign (segid 3A4 and resid 103 and name CB)	(segid 3A4 and resid 260 and name CA)	17.73	0.35	0.34
	assign (segid 3A4 and resid 103 and name CB)	(segid 3A4 and resid 260 and name CB)	18.18	0.55	0.55
	assign (segid 3A4 and resid 103 and name CB)	(segid 3A4 and resid 263 and name CA)	16.78	0.41	0.42
	assign (segid 3A4 and resid 103 and name CB)	(segid 3A4 and resid 263 and name CB)	15.53	0.38	0.37
	assign (segid 3A4 and resid 103 and name CB)	(segid 3A4 and resid 305 and name CB)	16.91	1.36	1.36
15	assign (segid 3A4 and resid 103 and name CB)	(segid 3A4 and resid 396 and name CA)	17.18	0.65	0.64
	assign (segid 3A4 and resid 103 and name CB)	(segid 3A4 and resid 396 and name CB)	17.41	0.77	0.77
	assign (segid 3A4 and resid 103 and name CB)	(segid 3A4 and resid 397 and name CA)	17.54	0.20	0.21
	assign (segid 3A4 and resid 103 and name CB)	(segid 3A4 and resid 397 and name CB)	18.89	0.16	0.17
20	assign (segid 3A4 and resid 103 and name CB)	(segid 3A4 and resid 398 and name CA)	17.57	0.33	0.33
	assign (segid 3A4 and resid 103 and name CB)	(segid 3A4 and resid 398 and name CB)	18.69	0.39	0.38
	assign (segid 3A4 and resid 103 and name CB)	(segid 3A4 and resid 399 and name CA)	14.53	0.46	0.47
	assign (segid 3A4 and resid 103 and name CB)	(segid 3A4 and resid 399 and name CB)	14.46	0.62	0.62
	assign (segid 3A4 and resid 103 and name CB)	(segid 3A4 and resid 400 and name CA)	12.54	0.19	0.19
	assign (segid 3A4 and resid 103 and name CB)	(segid 3A4 and resid 400 and name CB)	13.06	0.24	0.23
25	assign (segid 3A4 and resid 103 and name CB)	(segid 3A4 and resid 401 and name CA)	14.25	0.57	0.57
	assign (segid 3A4 and resid 103 and name CB)	(segid 3A4 and resid 402 and name CA)	13.89	0.60	0.60
	assign (segid 3A4 and resid 103 and name CB)	(segid 3A4 and resid 402 and name CB)	14.59	0.54	0.55
	assign (segid 3A4 and resid 103 and name CB)	(segid 3A4 and resid 403 and name CA)	10.23	0.61	0.61
	assign (segid 3A4 and resid 103 and name CB)	(segid 3A4 and resid 403 and name CB)	9.61	0.50	0.49
30	assign (segid 3A4 and resid 103 and name CB)	(segid 3A4 and resid 404 and name CA)	9.86	0.83	0.83
	assign (segid 3A4 and resid 103 and name CB)	(segid 3A4 and resid 404 and name CB)	10.62	0.73	0.73
	assign (segid 3A4 and resid 103 and name CB)	(segid 3A4 and resid 405 and name CA)	12.67	1.11	1.12
	assign (segid 3A4 and resid 103 and name CB)	(segid 3A4 and resid 405 and name CB)	14.06	1.06	1.06
	assign (segid 3A4 and resid 103 and name CB)	(segid 3A4 and resid 406 and name CA)	11.90	1.29	1.29
35	assign (segid 3A4 and resid 103 and name CB)	(segid 3A4 and resid 407 and name CA)	8.71	1.50	1.49
	assign (segid 3A4 and resid 103 and name CB)	(segid 3A4 and resid 407 and name CB)	7.34	1.46	1.46
	assign (segid 3A4 and resid 103 and name CB)	(segid 3A4 and resid 408 and name CA)	10.57	1.57	1.57
	assign (segid 3A4 and resid 103 and name CB)	(segid 3A4 and resid 408 and name CB)	11.36	1.52	1.52
	assign (segid 3A4 and resid 103 and name CB)	(segid 3A4 and resid 409 and name CA)	13.64	1.59	1.59
40	assign (segid 3A4 and resid 103 and name CB)	(segid 3A4 and resid 409 and name CB)	14.65	1.53	1.53
	assign (segid 3A4 and resid 103 and name CB)	(segid 3A4 and resid 410 and name CA)	12.50	1.66	1.65
	assign (segid 3A4 and resid 103 and name CB)	(segid 3A4 and resid 411 and name CA)	11.34	1.69	1.68
	assign (segid 3A4 and resid 103 and name CB)	(segid 3A4 and resid 411 and name CB)	10.06	1.68	1.69
	assign (segid 3A4 and resid 103 and name CB)	(segid 3A4 and resid 412 and name CA)	14.27	1.75	1.75
45	assign (segid 3A4 and resid 103 and name N)	(segid 3A4 and resid 103 and name C)	2.46	0.05	0.04
	assign (segid 3A4 and resid 103 and name N)	(segid 3A4 and resid 103 and name CA)	1.47	0.01	0.01
	assign (segid 3A4 and resid 103 and name N)	(segid 3A4 and resid 103 and name CB)	2.45	0.04	0.04
	assign (segid 3A4 and resid 103 and name N)	(segid 3A4 and resid 103 and name O)	3.49	0.06	0.06
	assign (segid 3A4 and resid 103 and name N)	(segid 3A4 and resid 104 and name C)	4.68	0.07	0.07
50	assign (segid 3A4 and resid 103 and name N)	(segid 3A4 and resid 104 and name CA)	4.20	0.03	0.04
	assign (segid 3A4 and resid 103 and name N)	(segid 3A4 and resid 104 and name CB)	4.95	0.04	0.03
	assign (segid 3A4 and resid 103 and name N)	(segid 3A4 and resid 104 and name N)	2.81	0.03	0.04
	assign (segid 3A4 and resid 103 and name N)	(segid 3A4 and resid 104 and name O)	5.76	0.09	0.09
	assign (segid 3A4 and resid 103 and name N)	(segid 3A4 and resid 105 and name C)	5.62	0.09	0.09
55	assign (segid 3A4 and resid 103 and name N)	(segid 3A4 and resid 105 and name CA)	5.30	0.09	0.09
	assign (segid 3A4 and resid 103 and name N)	(segid 3A4 and resid 105 and name CB)	5.35	0.12	0.13
	assign (segid 3A4 and resid 103 and name N)	(segid 3A4 and resid 105 and name N)	4.29	0.08	0.09
	assign (segid 3A4 and resid 103 and name N)	(segid 3A4 and resid 105 and name O)	6.83	0.09	0.08
	assign (segid 3A4 and resid 103 and name N)	(segid 3A4 and resid 106 and name C)	6.47	0.10	0.09
60	assign (segid 3A4 and resid 103 and name N)	(segid 3A4 and resid 106 and name CA)	5.63	0.08	0.07
	assign (segid 3A4 and resid 103 and name N)	(segid 3A4 and resid 106 and name CB)	5.09	0.07	0.08
	assign (segid 3A4 and resid 103 and name N)	(segid 3A4 and resid 106 and name N)	4.81	0.08	0.09
	assign (segid 3A4 and resid 103 and name N)	(segid 3A4 and resid 106 and name O)	7.68	0.09	0.09
	assign (segid 3A4 and resid 103 and name N)	(segid 3A4 and resid 107 and name CA)	7.17	0.12	0.12
65	assign (segid 3A4 and resid 103 and name N)	(segid 3A4 and resid 107 and name CB)	6.95	0.11	0.10
	assign (segid 3A4 and resid 103 and name N)	(segid 3A4 and resid 107 and name N)	6.05	0.12	0.11
	assign (segid 3A4 and resid 103 and name O)	(segid 3A4 and resid 103 and name CB)	3.29	0.03	0.02
	assign (segid 3A4 and resid 103 and name O)	(segid 3A4 and resid 104 and name C)	2.96	0.07	0.06
	assign (segid 3A4 and resid 103 and name O)	(segid 3A4 and resid 104 and name CA)	2.75	0.03	0.04
70	assign (segid 3A4 and resid 103 and name O)	(segid 3A4 and resid 104 and name CB)	4.24	0.03	0.03
	assign (segid 3A4 and resid 103 and name O)	(segid 3A4 and resid 104 and name N)	2.23	0.02	0.03
	assign (segid 3A4 and resid 103 and name O)	(segid 3A4 and resid 104 and name O)	3.42	0.12	0.11
	assign (segid 3A4 and resid 103 and name O)	(segid 3A4 and resid 105 and name C)	4.13	0.12	0.13
	assign (segid 3A4 and resid 103 and name O)	(segid 3A4 and resid 105 and name CA)	4.38	0.11	0.12
75	assign (segid 3A4 and resid 103 and name O)	(segid 3A4 and resid 105 and name CB)	5.36	0.15	0.15
	assign (segid 3A4 and resid 103 and name O)	(segid 3A4 and resid 105 and name N)	3.43	0.11	0.10
	assign (segid 3A4 and resid 103 and name O)	(segid 3A4 and resid 105 and name O)	5.05	0.15	0.15
	assign (segid 3A4 and resid 103 and name O)	(segid 3A4 and resid 106 and name C)	3.88	0.08	0.08
	assign (segid 3A4 and resid 103 and name O)	(segid 3A4 and resid 106 and name CA)	3.85	0.09	0.10
80	assign (segid 3A4 and resid 103 and name O)	(segid 3A4 and resid 106 and name CB)	3.78	0.12	0.12
	assign (segid 3A4 and resid 103 and name O)	(segid 3A4 and resid 106 and name N)	3.34	0.10	0.10
	assign (segid 3A4 and resid 103 and name O)	(segid 3A4 and resid 106 and name O)	5.07	0.09	0.08
	assign (segid 3A4 and resid 103 and name O)	(segid 3A4 and resid 107 and name C)	4.97	0.14	0.14

	assign (segid 3A4 and resid 103 and name O)	(segid 3A4 and resid 107 and name CA)	3.80	0.11	0.11
	assign (segid 3A4 and resid 103 and name O)	(segid 3A4 and resid 107 and name CB)	3.47	0.10	0.11
	assign (segid 3A4 and resid 103 and name O)	(segid 3A4 and resid 107 and name N)	2.98	0.10	0.09
	assign (segid 3A4 and resid 103 and name O)	(segid 3A4 and resid 107 and name O)	6.09	0.14	0.13
	assign (segid 3A4 and resid 103 and name O)	(segid 3A4 and resid 108 and name C)	7.23	0.12	0.12
5	assign (segid 3A4 and resid 103 and name O)	(segid 3A4 and resid 108 and name CA)	6.37	0.15	0.15
	assign (segid 3A4 and resid 103 and name O)	(segid 3A4 and resid 108 and name CB)	6.59	0.19	0.19
	assign (segid 3A4 and resid 103 and name O)	(segid 3A4 and resid 108 and name N)	5.01	0.13	0.14
	assign (segid 3A4 and resid 103 and name O)	(segid 3A4 and resid 109 and name N)	6.92	0.14	0.13
	assign (segid 3A4 and resid 103 and name O)	(segid 3A4 and resid 110 and name CB)	7.64	0.06	0.05
10	assign (segid 3A4 and resid 103 and name O)	(segid 3A4 and resid 110 and name N)	7.70	0.06	0.06
	assign (segid 3A4 and resid 104 and name C)	(segid 3A4 and resid 104 and name CB)	2.48	0.02	0.03
	assign (segid 3A4 and resid 104 and name C)	(segid 3A4 and resid 104 and name O)	1.23	0.01	0.01
	assign (segid 3A4 and resid 104 and name C)	(segid 3A4 and resid 105 and name C)	3.06	0.03	0.04
	assign (segid 3A4 and resid 104 and name C)	(segid 3A4 and resid 105 and name CA)	2.45	0.02	0.01
15	assign (segid 3A4 and resid 104 and name C)	(segid 3A4 and resid 105 and name CB)	3.71	0.02	0.02
	assign (segid 3A4 and resid 104 and name C)	(segid 3A4 and resid 105 and name N)	1.33	0.01	0.00
	assign (segid 3A4 and resid 104 and name C)	(segid 3A4 and resid 105 and name O)	3.90	0.09	0.09
	assign (segid 3A4 and resid 104 and name C)	(segid 3A4 and resid 106 and name C)	4.59	0.03	0.03
	assign (segid 3A4 and resid 104 and name C)	(segid 3A4 and resid 106 and name CA)	4.53	0.03	0.04
20	assign (segid 3A4 and resid 104 and name C)	(segid 3A4 and resid 106 and name CB)	5.31	0.08	0.07
	assign (segid 3A4 and resid 104 and name C)	(segid 3A4 and resid 106 and name N)	3.33	0.03	0.03
	assign (segid 3A4 and resid 104 and name C)	(segid 3A4 and resid 106 and name O)	5.61	0.06	0.05
	assign (segid 3A4 and resid 104 and name C)	(segid 3A4 and resid 107 and name C)	4.92	0.09	0.08
	assign (segid 3A4 and resid 104 and name C)	(segid 3A4 and resid 107 and name CA)	4.57	0.04	0.04
25	assign (segid 3A4 and resid 104 and name C)	(segid 3A4 and resid 107 and name CB)	4.36	0.10	0.10
	assign (segid 3A4 and resid 104 and name C)	(segid 3A4 and resid 107 and name N)	3.87	0.04	0.03
	assign (segid 3A4 and resid 104 and name C)	(segid 3A4 and resid 107 and name O)	6.12	0.09	0.09
	assign (segid 3A4 and resid 104 and name C)	(segid 3A4 and resid 108 and name C)	6.17	0.08	0.08
	assign (segid 3A4 and resid 104 and name C)	(segid 3A4 and resid 108 and name CA)	5.09	0.08	0.08
30	assign (segid 3A4 and resid 104 and name C)	(segid 3A4 and resid 108 and name CB)	4.66	0.13	0.13
	assign (segid 3A4 and resid 104 and name C)	(segid 3A4 and resid 108 and name N)	4.20	0.08	0.07
	assign (segid 3A4 and resid 104 and name C)	(segid 3A4 and resid 108 and name O)	7.31	0.08	0.09
	assign (segid 3A4 and resid 104 and name C)	(segid 3A4 and resid 109 and name CA)	7.36	0.16	0.16
35	assign (segid 3A4 and resid 104 and name C)	(segid 3A4 and resid 109 and name CB)	7.39	0.19	0.19
	assign (segid 3A4 and resid 104 and name C)	(segid 3A4 and resid 109 and name N)	6.08	0.13	0.13
	assign (segid 3A4 and resid 104 and name C)	(segid 3A4 and resid 109 and name O)	1.51	0.00	0.01
	assign (segid 3A4 and resid 104 and name CA)	(segid 3A4 and resid 104 and name CB)	1.53	0.01	0.01
	assign (segid 3A4 and resid 104 and name CA)	(segid 3A4 and resid 104 and name O)	2.39	0.03	0.03
	assign (segid 3A4 and resid 104 and name CA)	(segid 3A4 and resid 105 and name C)	4.45	0.04	0.03
40	assign (segid 3A4 and resid 104 and name CA)	(segid 3A4 and resid 105 and name CB)	3.82	0.02	0.01
	assign (segid 3A4 and resid 104 and name CA)	(segid 3A4 and resid 105 and name N)	4.86	0.06	0.06
	assign (segid 3A4 and resid 104 and name CA)	(segid 3A4 and resid 105 and name O)	2.44	0.02	0.03
	assign (segid 3A4 and resid 104 and name CA)	(segid 3A4 and resid 106 and name C)	5.55	0.04	0.03
45	assign (segid 3A4 and resid 104 and name CA)	(segid 3A4 and resid 106 and name CA)	5.53	0.04	0.03
	assign (segid 3A4 and resid 104 and name CA)	(segid 3A4 and resid 106 and name CB)	5.98	0.09	0.08
	assign (segid 3A4 and resid 104 and name CA)	(segid 3A4 and resid 106 and name N)	4.42	0.03	0.04
	assign (segid 3A4 and resid 104 and name CA)	(segid 3A4 and resid 106 and name O)	6.64	0.06	0.05
50	assign (segid 3A4 and resid 104 and name CA)	(segid 3A4 and resid 107 and name C)	5.74	0.09	0.09
	assign (segid 3A4 and resid 104 and name CA)	(segid 3A4 and resid 107 and name CA)	5.15	0.05	0.05
	assign (segid 3A4 and resid 104 and name CA)	(segid 3A4 and resid 107 and name CB)	4.52	0.09	0.10
	assign (segid 3A4 and resid 104 and name CA)	(segid 3A4 and resid 107 and name N)	4.61	0.04	0.04
	assign (segid 3A4 and resid 104 and name CA)	(segid 3A4 and resid 107 and name O)	6.93	0.10	0.10
55	assign (segid 3A4 and resid 104 and name CA)	(segid 3A4 and resid 108 and name C)	7.41	0.09	0.08
	assign (segid 3A4 and resid 104 and name CA)	(segid 3A4 and resid 108 and name CA)	6.21	0.09	0.08
	assign (segid 3A4 and resid 104 and name CA)	(segid 3A4 and resid 108 and name CB)	5.87	0.14	0.14
	assign (segid 3A4 and resid 104 and name CA)	(segid 3A4 and resid 108 and name N)	5.22	0.08	0.08
	assign (segid 3A4 and resid 104 and name CA)	(segid 3A4 and resid 109 and name CA)	8.71	0.15	0.15
60	assign (segid 3A4 and resid 104 and name CA)	(segid 3A4 and resid 109 and name CB)	8.78	0.18	0.18
	assign (segid 3A4 and resid 104 and name CA)	(segid 3A4 and resid 109 and name N)	7.40	0.13	0.13
	assign (segid 3A4 and resid 104 and name CA)	(segid 3A4 and resid 110 and name CA)	9.86	0.11	0.10
	assign (segid 3A4 and resid 104 and name CA)	(segid 3A4 and resid 110 and name CB)	9.34	0.11	0.11
	assign (segid 3A4 and resid 104 and name CA)	(segid 3A4 and resid 111 and name CA)	11.00	0.53	0.53
65	assign (segid 3A4 and resid 104 and name CA)	(segid 3A4 and resid 111 and name CB)	10.34	0.67	0.68
	assign (segid 3A4 and resid 104 and name CA)	(segid 3A4 and resid 112 and name CA)	13.22	0.30	0.30
	assign (segid 3A4 and resid 104 and name CA)	(segid 3A4 and resid 119 and name CA)	16.10	1.11	1.11
	assign (segid 3A4 and resid 104 and name CA)	(segid 3A4 and resid 119 and name CB)	14.78	0.99	0.99
	assign (segid 3A4 and resid 104 and name CA)	(segid 3A4 and resid 120 and name CA)	16.67	0.56	0.57
70	assign (segid 3A4 and resid 104 and name CA)	(segid 3A4 and resid 120 and name CB)	17.25	0.67	0.67
	assign (segid 3A4 and resid 104 and name CA)	(segid 3A4 and resid 121 and name CA)	14.54	0.16	0.16
	assign (segid 3A4 and resid 104 and name CA)	(segid 3A4 and resid 121 and name CB)	15.03	0.27	0.27
	assign (segid 3A4 and resid 104 and name CA)	(segid 3A4 and resid 122 and name CA)	15.62	0.40	0.41
	assign (segid 3A4 and resid 104 and name CA)	(segid 3A4 and resid 122 and name CB)	17.09	0.43	0.43
75	assign (segid 3A4 and resid 104 and name CA)	(segid 3A4 and resid 123 and name CA)	14.62	0.38	0.38
	assign (segid 3A4 and resid 104 and name CA)	(segid 3A4 and resid 123 and name CB)	15.44	0.70	0.70
	assign (segid 3A4 and resid 104 and name CA)	(segid 3A4 and resid 124 and name CA)	11.37	0.64	0.64
	assign (segid 3A4 and resid 104 and name CA)	(segid 3A4 and resid 124 and name CB)	11.35	1.07	1.01
	assign (segid 3A4 and resid 104 and name CA)	(segid 3A4 and resid 125 and name CA)	10.49	0.57	0.57
80	assign (segid 3A4 and resid 104 and name CA)	(segid 3A4 and resid 125 and name CB)	10.90	1.01	1.01
	assign (segid 3A4 and resid 104 and name CA)	(segid 3A4 and resid 126 and name CA)	12.59	0.61	0.62
	assign (segid 3A4 and resid 104 and name CA)	(segid 3A4 and resid 127 and name CA)	12.23	1.35	1.35
	assign (segid 3A4 and resid 104 and name CA)	(segid 3A4 and resid 127 and name CB)	12.53	1.93	1.93

	assign (segid 3A4 and resid 104 and name CA) (segid 3A4 and resid 128 and name CA)	9.65	0.99	1.00
	assign (segid 3A4 and resid 104 and name CA) (segid 3A4 and resid 128 and name CB)	9.02	0.71	0.70
	assign (segid 3A4 and resid 104 and name CA) (segid 3A4 and resid 129 and name CA)	9.74	1.38	1.37
	assign (segid 3A4 and resid 104 and name CA) (segid 3A4 and resid 129 and name CB)	10.05	1.77	1.77
5	assign (segid 3A4 and resid 104 and name CA) (segid 3A4 and resid 130 and name CA)	12.32	1.02	1.02
	assign (segid 3A4 and resid 104 and name CA) (segid 3A4 and resid 130 and name CB)	13.21	0.93	0.93
	assign (segid 3A4 and resid 104 and name CA) (segid 3A4 and resid 131 and name CA)	12.11	1.48	1.48
	assign (segid 3A4 and resid 104 and name CA) (segid 3A4 and resid 131 and name CB)	11.87	2.02	2.02
	assign (segid 3A4 and resid 104 and name CA) (segid 3A4 and resid 132 and name CA)	10.63	1.14	1.15
	assign (segid 3A4 and resid 104 and name CA) (segid 3A4 and resid 132 and name CB)	9.72	1.35	1.35
10	assign (segid 3A4 and resid 104 and name CA) (segid 3A4 and resid 133 and name CA)	12.37	1.82	1.81
	assign (segid 3A4 and resid 104 and name CA) (segid 3A4 and resid 133 and name CB)	12.62	2.08	2.07
	assign (segid 3A4 and resid 104 and name CA) (segid 3A4 and resid 134 and name CA)	14.72	1.29	1.29
	assign (segid 3A4 and resid 104 and name CA) (segid 3A4 and resid 135 and name CA)	14.36	1.41	1.41
	assign (segid 3A4 and resid 104 and name CA) (segid 3A4 and resid 135 and name CB)	13.54	1.58	1.59
15	assign (segid 3A4 and resid 104 and name CA) (segid 3A4 and resid 136 and name CA)	14.45	1.36	1.37
	assign (segid 3A4 and resid 104 and name CA) (segid 3A4 and resid 136 and name CB)	13.64	1.71	1.71
	assign (segid 3A4 and resid 104 and name CA) (segid 3A4 and resid 137 and name CA)	16.98	1.46	1.46
	assign (segid 3A4 and resid 104 and name CA) (segid 3A4 and resid 141 and name CA)	14.98	2.43	2.43
	assign (segid 3A4 and resid 104 and name CA) (segid 3A4 and resid 256 and name CA)	17.45	1.48	1.48
20	assign (segid 3A4 and resid 104 and name CA) (segid 3A4 and resid 259 and name CA)	17.03	0.96	0.96
	assign (segid 3A4 and resid 104 and name CA) (segid 3A4 and resid 259 and name CB)	16.11	1.03	1.03
	assign (segid 3A4 and resid 104 and name CA) (segid 3A4 and resid 260 and name CA)	15.86	0.78	0.78
	assign (segid 3A4 and resid 104 and name CA) (segid 3A4 and resid 260 and name CB)	16.00	0.91	0.92
	assign (segid 3A4 and resid 104 and name CA) (segid 3A4 and resid 263 and name CA)	15.83	0.65	0.64
25	assign (segid 3A4 and resid 104 and name CA) (segid 3A4 and resid 263 and name CB)	14.43	0.67	0.67
	assign (segid 3A4 and resid 104 and name CA) (segid 3A4 and resid 264 and name CA)	17.44	0.53	0.53
	assign (segid 3A4 and resid 104 and name CA) (segid 3A4 and resid 267 and name CA)	18.11	0.23	0.24
	assign (segid 3A4 and resid 104 and name CA) (segid 3A4 and resid 267 and name CB)	16.96	0.26	0.26
	assign (segid 3A4 and resid 104 and name CA) (segid 3A4 and resid 296 and name CA)	17.81	1.29	1.30
30	assign (segid 3A4 and resid 104 and name CA) (segid 3A4 and resid 396 and name CB)	17.79	1.38	1.38
	assign (segid 3A4 and resid 104 and name CA) (segid 3A4 and resid 397 and name CA)	17.73	1.00	1.01
	assign (segid 3A4 and resid 104 and name CA) (segid 3A4 and resid 398 and name CA)	18.51	0.96	0.96
	assign (segid 3A4 and resid 104 and name CA) (segid 3A4 and resid 399 and name CA)	15.94	1.14	1.14
35	assign (segid 3A4 and resid 104 and name CA) (segid 3A4 and resid 399 and name CB)	15.93	1.28	1.28
	assign (segid 3A4 and resid 104 and name CA) (segid 3A4 and resid 400 and name CA)	13.11	0.95	0.96
	assign (segid 3A4 and resid 104 and name CA) (segid 3A4 and resid 400 and name CB)	13.19	0.97	0.97
	assign (segid 3A4 and resid 104 and name CA) (segid 3A4 and resid 401 and name CA)	14.77	0.67	0.67
	assign (segid 3A4 and resid 104 and name CA) (segid 3A4 and resid 402 and name CA)	15.43	0.69	0.70
40	assign (segid 3A4 and resid 104 and name CA) (segid 3A4 and resid 402 and name CB)	16.39	0.82	0.81
	assign (segid 3A4 and resid 104 and name CA) (segid 3A4 and resid 403 and name CA)	12.09	0.72	0.73
	assign (segid 3A4 and resid 104 and name CA) (segid 3A4 and resid 403 and name CB)	11.45	0.89	0.89
	assign (segid 3A4 and resid 104 and name CA) (segid 3A4 and resid 404 and name CA)	10.60	0.58	0.59
	assign (segid 3A4 and resid 104 and name CA) (segid 3A4 and resid 404 and name CB)	10.83	0.73	0.73
45	assign (segid 3A4 and resid 104 and name CA) (segid 3A4 and resid 405 and name CA)	13.66	0.56	0.55
	assign (segid 3A4 and resid 104 and name CA) (segid 3A4 and resid 405 and name CB)	15.02	0.56	0.57
	assign (segid 3A4 and resid 104 and name CA) (segid 3A4 and resid 406 and name CA)	13.96	0.47	0.46
	assign (segid 3A4 and resid 104 and name CA) (segid 3A4 and resid 407 and name CA)	10.73	0.51	0.52
	assign (segid 3A4 and resid 104 and name CA) (segid 3A4 and resid 407 and name CB)	9.40	0.50	0.50
50	assign (segid 3A4 and resid 104 and name CA) (segid 3A4 and resid 408 and name CA)	11.29	0.51	0.51
	assign (segid 3A4 and resid 104 and name CA) (segid 3A4 and resid 408 and name CB)	11.66	0.59	0.59
	assign (segid 3A4 and resid 104 and name CA) (segid 3A4 and resid 409 and name CA)	14.82	0.49	0.49
	assign (segid 3A4 and resid 104 and name CA) (segid 3A4 and resid 409 and name CB)	15.92	0.42	0.43
	assign (segid 3A4 and resid 104 and name CA) (segid 3A4 and resid 410 and name CA)	14.46	0.69	0.70
55	assign (segid 3A4 and resid 104 and name CA) (segid 3A4 and resid 411 and name CA)	12.55	0.87	0.88
	assign (segid 3A4 and resid 104 and name CA) (segid 3A4 and resid 411 and name CB)	11.10	0.88	0.88
	assign (segid 3A4 and resid 104 and name CA) (segid 3A4 and resid 412 and name CA)	14.67	1.01	1.01
	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 105 and name C)	5.45	0.04	0.05
	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 105 and name CB)	4.47	0.02	0.02
60	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 105 and name N)	5.31	0.06	0.07
	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 105 and name O)	3.15	0.02	0.03
	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 106 and name C)	6.31	0.09	0.09
	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 106 and name CA)	6.95	0.05	0.05
	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 106 and name CB)	6.88	0.03	0.02
65	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 106 and name N)	7.39	0.08	0.07
	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 107 and name C)	5.65	0.02	0.02
	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 107 and name CA)	6.92	0.11	0.10
	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 107 and name CB)	6.52	0.08	0.07
	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 107 and name N)	5.81	0.13	0.13
70	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 108 and name CA)	6.05	0.05	0.05
	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 108 and name CB)	7.00	0.08	0.08
	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 108 and name N)	6.39	0.10	0.11
	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 109 and name CA)	6.24	0.11	0.10
	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 109 and name CB)	9.73	0.17	0.16
75	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 109 and name N)	9.84	0.19	0.18
	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 110 and name CA)	11.14	0.14	0.14
	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 110 and name CB)	10.70	0.14	0.15
	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 111 and name CA)	12.00	0.62	0.62
	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 111 and name CB)	11.22	0.77	0.77
80	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 112 and name CA)	14.12	0.39	0.39
	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 119 and name CA)	16.75	1.06	1.07
	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 119 and name CB)	15.47	0.91	0.92
	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 120 and name CA)	17.08	0.61	0.61

	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 120 and name CB)	17.55	0.75	0.76
	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 121 and name CA)	14.98	0.21	0.22
	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 121 and name CB)	15.55	0.31	0.30
	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 122 and name CA)	15.72	0.54	0.55
	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 122 and name CB)	17.15	0.60	0.60
5	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 123 and name CA)	14.54	0.58	0.59
	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 123 and name CB)	15.38	0.86	0.85
	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 124 and name CA)	11.49	0.83	0.82
	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 124 and name CB)	11.64	1.17	1.17
	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 125 and name CA)	10.62	0.45	0.46
10	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 125 and name CB)	11.20	0.79	0.79
	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 126 and name CA)	12.44	0.75	0.76
	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 127 and name CA)	11.76	1.65	1.65
	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 127 and name CB)	12.08	2.18	2.18
	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 128 and name CA)	9.10	1.14	1.14
15	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 128 and name CB)	8.60	0.77	0.78
	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 129 and name CA)	9.19	1.41	1.42
	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 129 and name CB)	9.68	1.71	1.72
	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 130 and name CA)	11.53	1.26	1.27
	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 130 and name CB)	12.47	1.26	1.26
20	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 131 and name CA)	11.10	1.75	1.75
	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 131 and name CB)	10.87	2.29	2.29
	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 132 and name CA)	9.58	1.28	1.28
	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 132 and name CB)	8.73	1.46	1.47
	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 133 and name CA)	11.30	1.92	1.93
25	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 133 and name CB)	11.64	2.14	2.15
	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 134 and name CA)	13.57	1.50	1.49
	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 135 and name CA)	13.14	1.51	1.51
	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 135 and name CB)	12.34	1.65	1.65
	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 136 and name CA)	13.26	1.40	1.41
30	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 136 and name CB)	12.50	1.77	1.77
	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 137 and name CA)	15.80	1.52	1.51
	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 138 and name CA)	17.50	1.41	1.41
	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 138 and name CB)	17.63	1.50	1.50
	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 139 and name CA)	16.37	1.50	1.51
35	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 140 and name CA)	15.45	1.91	1.91
	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 140 and name CB)	15.71	1.83	1.83
	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 141 and name CA)	13.61	2.68	2.49
	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 141 and name CB)	14.04	3.24	3.24
	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 147 and name CA)	14.57	2.21	2.21
40	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 147 and name CB)	16.43	1.75	1.74
	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 150 and name CA)	15.56	2.10	2.11
	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 256 and name CA)	16.70	1.76	1.76
	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 259 and name CA)	16.69	1.28	1.29
	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 259 and name CB)	15.71	1.35	1.34
45	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 260 and name CA)	15.61	1.07	1.08
	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 260 and name CB)	15.67	1.18	1.18
	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 263 and name CA)	16.03	0.95	0.95
	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 263 and name CB)	14.59	0.97	0.96
	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 264 and name CA)	17.70	0.83	0.83
50	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 267 and name CA)	18.76	0.48	0.48
	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 267 and name CB)	17.60	0.46	0.46
	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 396 and name CA)	17.32	1.53	1.53
	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 396 and name CB)	17.18	1.60	1.61
	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 397 and name CA)	17.38	1.28	1.29
55	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 398 and name CA)	18.41	1.22	1.22
	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 399 and name CA)	15.85	1.36	1.35
	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 399 and name CB)	15.74	1.49	1.49
	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 400 and name CA)	12.97	1.20	1.20
	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 400 and name CB)	12.92	1.23	1.23
60	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 401 and name CA)	14.91	0.93	0.93
	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 402 and name CA)	15.78	0.90	0.91
	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 402 and name CB)	16.69	1.01	1.02
	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 403 and name CA)	12.50	0.88	0.88
	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 403 and name CB)	11.72	1.03	1.02
65	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 404 and name CA)	11.12	0.78	0.78
	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 404 and name CB)	11.22	0.97	0.96
	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 405 and name CA)	14.36	0.70	0.70
	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 405 and name CB)	15.67	0.74	0.73
	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 406 and name CA)	14.80	0.53	0.54
70	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 407 and name CA)	11.77	0.51	0.50
	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 407 and name CB)	10.38	0.51	0.52
	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 408 and name CA)	12.39	0.38	0.38
	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 408 and name CB)	12.66	0.50	0.49
	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 409 and name CA)	15.97	0.33	0.34
75	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 409 and name CB)	17.02	0.32	0.32
	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 410 and name CA)	15.73	0.59	0.60
	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 411 and name CA)	13.95	0.76	0.76
	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 411 and name CB)	12.50	0.77	0.76
	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 412 and name CA)	16.01	0.86	0.86
80	assign (segid 3A4 and resid 104 and name CB) (segid 3A4 and resid 104 and name C)	2.45	0.04	0.04
	assign (segid 3A4 and resid 104 and name N) (segid 3A4 and resid 104 and name CA)	1.46	0.01	0.00
	assign (segid 3A4 and resid 104 and name N) (segid 3A4 and resid 104 and name CB)	2.45	0.01	0.01

	assign (segid 3A4 and resid 104 and name N) (segid 3A4 and resid 104 and name O)	3.48	0.07	0.07
	assign (segid 3A4 and resid 104 and name N) (segid 3A4 and resid 105 and name C)	4.73	0.03	0.04
	assign (segid 3A4 and resid 104 and name N) (segid 3A4 and resid 105 and name CA)	4.22	0.02	0.03
	assign (segid 3A4 and resid 104 and name N) (segid 3A4 and resid 105 and name CB)	4.97	0.05	0.05
5	assign (segid 3A4 and resid 104 and name N) (segid 3A4 and resid 105 and name N)	2.82	0.03	0.03
	assign (segid 3A4 and resid 104 and name N) (segid 3A4 and resid 105 and name O)	5.81	0.05	0.05
	assign (segid 3A4 and resid 104 and name N) (segid 3A4 and resid 106 and name C)	5.66	0.03	0.03
	assign (segid 3A4 and resid 104 and name N) (segid 3A4 and resid 106 and name CA)	5.38	0.03	0.04
	assign (segid 3A4 and resid 104 and name N) (segid 3A4 and resid 106 and name CB)	5.47	0.08	0.07
10	assign (segid 3A4 and resid 104 and name N) (segid 3A4 and resid 106 and name N)	4.35	0.05	0.05
	assign (segid 3A4 and resid 104 and name N) (segid 3A4 and resid 106 and name O)	6.86	0.04	0.03
	assign (segid 3A4 and resid 104 and name N) (segid 3A4 and resid 107 and name C)	6.45	0.09	0.10
	assign (segid 3A4 and resid 104 and name N) (segid 3A4 and resid 107 and name CA)	5.59	0.07	0.06
	assign (segid 3A4 and resid 104 and name N) (segid 3A4 and resid 107 and name CB)	5.03	0.06	0.06
15	assign (segid 3A4 and resid 104 and name N) (segid 3A4 and resid 107 and name N)	4.82	0.05	0.06
	assign (segid 3A4 and resid 104 and name N) (segid 3A4 and resid 107 and name O)	7.65	0.10	0.10
	assign (segid 3A4 and resid 104 and name N) (segid 3A4 and resid 108 and name C)	7.24	0.08	0.09
	assign (segid 3A4 and resid 104 and name N) (segid 3A4 and resid 108 and name CB)	7.02	0.14	0.14
	assign (segid 3A4 and resid 104 and name N) (segid 3A4 and resid 108 and name N)	6.11	0.07	0.08
20	assign (segid 3A4 and resid 104 and name N) (segid 3A4 and resid 104 and name O)	3.29	0.06	0.06
	assign (segid 3A4 and resid 104 and name O) (segid 3A4 and resid 105 and name C)	3.02	0.07	0.06
	assign (segid 3A4 and resid 104 and name O) (segid 3A4 and resid 105 and name CA)	2.77	0.02	0.01
	assign (segid 3A4 and resid 104 and name O) (segid 3A4 and resid 105 and name CB)	4.24	0.02	0.03
	assign (segid 3A4 and resid 104 and name O) (segid 3A4 and resid 105 and name N)	2.23	0.02	0.02
25	assign (segid 3A4 and resid 104 and name O) (segid 3A4 and resid 105 and name O)	3.48	0.13	0.14
	assign (segid 3A4 and resid 104 and name O) (segid 3A4 and resid 106 and name C)	4.17	0.07	0.06
	assign (segid 3A4 and resid 104 and name O) (segid 3A4 and resid 106 and name CA)	4.47	0.06	0.06
	assign (segid 3A4 and resid 104 and name O) (segid 3A4 and resid 106 and name CB)	5.46	0.08	0.09
	assign (segid 3A4 and resid 104 and name O) (segid 3A4 and resid 106 and name N)	3.49	0.06	0.06
30	assign (segid 3A4 and resid 104 and name O) (segid 3A4 and resid 106 and name O)	5.01	0.08	0.08
	assign (segid 3A4 and resid 104 and name O) (segid 3A4 and resid 107 and name C)	3.89	0.08	0.08
	assign (segid 3A4 and resid 104 and name O) (segid 3A4 and resid 107 and name CA)	3.82	0.08	0.09
	assign (segid 3A4 and resid 104 and name O) (segid 3A4 and resid 107 and name CB)	3.70	0.15	0.15
	assign (segid 3A4 and resid 104 and name O) (segid 3A4 and resid 107 and name N)	3.39	0.08	0.08
35	assign (segid 3A4 and resid 104 and name O) (segid 3A4 and resid 107 and name O)	5.07	0.09	0.09
	assign (segid 3A4 and resid 104 and name O) (segid 3A4 and resid 108 and name C)	5.07	0.10	0.09
	assign (segid 3A4 and resid 104 and name O) (segid 3A4 and resid 108 and name CA)	3.90	0.09	0.09
	assign (segid 3A4 and resid 104 and name O) (segid 3A4 and resid 108 and name CB)	3.56	0.16	0.16
	assign (segid 3A4 and resid 104 and name O) (segid 3A4 and resid 108 and name N)	3.06	0.06	0.07
40	assign (segid 3A4 and resid 104 and name O) (segid 3A4 and resid 108 and name O)	6.18	0.10	0.10
	assign (segid 3A4 and resid 104 and name O) (segid 3A4 and resid 109 and name C)	7.31	0.10	0.10
	assign (segid 3A4 and resid 104 and name O) (segid 3A4 and resid 109 and name CA)	6.48	0.15	0.15
	assign (segid 3A4 and resid 104 and name O) (segid 3A4 and resid 109 and name CB)	6.73	0.18	0.17
	assign (segid 3A4 and resid 104 and name O) (segid 3A4 and resid 109 and name N)	5.13	0.13	0.13
45	assign (segid 3A4 and resid 104 and name O) (segid 3A4 and resid 110 and name C)	7.74	0.10	0.10
	assign (segid 3A4 and resid 104 and name O) (segid 3A4 and resid 110 and name N)	6.94	0.12	0.12
	assign (segid 3A4 and resid 105 and name C) (segid 3A4 and resid 105 and name CB)	2.50	0.06	0.06
	assign (segid 3A4 and resid 105 and name C) (segid 3A4 and resid 105 and name O)	1.23	0.00	0.00
	assign (segid 3A4 and resid 105 and name C) (segid 3A4 and resid 106 and name C)	2.98	0.03	0.04
50	assign (segid 3A4 and resid 105 and name C) (segid 3A4 and resid 106 and name CA)	2.42	0.02	0.02
	assign (segid 3A4 and resid 105 and name C) (segid 3A4 and resid 106 and name CB)	3.71	0.02	0.01
	assign (segid 3A4 and resid 105 and name C) (segid 3A4 and resid 106 and name N)	1.33	0.01	0.00
	assign (segid 3A4 and resid 105 and name C) (segid 3A4 and resid 106 and name O)	3.76	0.05	0.04
	assign (segid 3A4 and resid 105 and name C) (segid 3A4 and resid 107 and name C)	4.58	0.07	0.07
55	assign (segid 3A4 and resid 105 and name C) (segid 3A4 and resid 107 and name CA)	4.46	0.04	0.05
	assign (segid 3A4 and resid 105 and name C) (segid 3A4 and resid 107 and name CB)	5.22	0.07	0.07
	assign (segid 3A4 and resid 105 and name C) (segid 3A4 and resid 107 and name N)	3.29	0.04	0.03
	assign (segid 3A4 and resid 105 and name C) (segid 3A4 and resid 107 and name O)	5.63	0.09	0.08
	assign (segid 3A4 and resid 105 and name C) (segid 3A4 and resid 108 and name C)	4.95	0.06	0.05
60	assign (segid 3A4 and resid 105 and name C) (segid 3A4 and resid 108 and name CA)	4.61	0.12	0.13
	assign (segid 3A4 and resid 105 and name C) (segid 3A4 and resid 108 and name CB)	4.38	0.23	0.24
	assign (segid 3A4 and resid 105 and name C) (segid 3A4 and resid 108 and name N)	3.90	0.12	0.12
	assign (segid 3A4 and resid 105 and name C) (segid 3A4 and resid 108 and name O)	6.14	0.06	0.07
	assign (segid 3A4 and resid 105 and name C) (segid 3A4 and resid 109 and name C)	6.19	0.11	0.11
65	assign (segid 3A4 and resid 105 and name C) (segid 3A4 and resid 109 and name CA)	5.16	0.15	0.14
	assign (segid 3A4 and resid 105 and name C) (segid 3A4 and resid 109 and name CB)	4.73	0.19	0.19
	assign (segid 3A4 and resid 105 and name C) (segid 3A4 and resid 109 and name N)	4.25	0.08	0.08
	assign (segid 3A4 and resid 105 and name C) (segid 3A4 and resid 109 and name O)	7.34	0.12	0.12
	assign (segid 3A4 and resid 105 and name C) (segid 3A4 and resid 110 and name CA)	7.28	0.07	0.08
70	assign (segid 3A4 and resid 105 and name C) (segid 3A4 and resid 110 and name CB)	7.28	0.05	0.05
	assign (segid 3A4 and resid 105 and name C) (segid 3A4 and resid 110 and name N)	6.04	0.09	0.09
	assign (segid 3A4 and resid 105 and name C) (segid 3A4 and resid 105 and name C)	1.52	0.01	0.01
	assign (segid 3A4 and resid 105 and name CA) (segid 3A4 and resid 105 and name CB)	1.53	0.02	0.02
	assign (segid 3A4 and resid 105 and name CA) (segid 3A4 and resid 105 and name O)	2.39	0.01	0.01
75	assign (segid 3A4 and resid 105 and name CA) (segid 3A4 and resid 106 and name C)	4.37	0.03	0.03
	assign (segid 3A4 and resid 105 and name CA) (segid 3A4 and resid 106 and name CA)	3.79	0.01	0.01
	assign (segid 3A4 and resid 105 and name CA) (segid 3A4 and resid 106 and name CB)	4.85	0.02	0.03
	assign (segid 3A4 and resid 105 and name CA) (segid 3A4 and resid 106 and name N)	2.42	0.01	0.02
	assign (segid 3A4 and resid 105 and name CA) (segid 3A4 and resid 106 and name O)	5.21	0.05	0.06
80	assign (segid 3A4 and resid 105 and name CA) (segid 3A4 and resid 107 and name C)	5.52	0.08	0.08
	assign (segid 3A4 and resid 105 and name CA) (segid 3A4 and resid 107 and name CA)	5.44	0.06	0.06
	assign (segid 3A4 and resid 105 and name CA) (segid 3A4 and resid 107 and name CB)	5.86	0.10	0.11
	assign (segid 3A4 and resid 105 and name CA) (segid 3A4 and resid 107 and name N)	4.37	0.03	0.03

	assign (segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 107 and name O)	6.64	0.08	0.08
	assign (segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 108 and name C)	5.80	0.05	0.06
	assign (segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 108 and name CA)	5.21	0.14	0.14
	assign (segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 108 and name CB)	4.58	0.24	0.25
5	assign (segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 108 and name N)	4.64	0.13	0.12
	assign (segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 108 and name O)	6.96	0.08	0.08
	assign (segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 109 and name C)	7.48	0.11	0.11
	assign (segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 109 and name CA)	6.33	0.15	0.14
	assign (segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 109 and name CB)	5.98	0.18	0.17
	assign (segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 109 and name N)	5.33	0.09	0.09
10	assign (segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 110 and name CA)	8.66	0.07	0.07
	assign (segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 110 and name CB)	8.65	0.04	0.05
	assign (segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 110 and name N)	7.40	0.10	0.09
	assign (segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 111 and name CA)	10.28	0.45	0.46
	assign (segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 111 and name CB)	9.97	0.61	0.61
15	assign (segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 112 and name CA)	11.51	0.26	0.27
	assign (segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 119 and name CA)	13.05	1.40	1.39
	assign (segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 119 and name CB)	11.74	1.32	1.31
	assign (segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 120 and name CA)	13.40	0.89	0.89
	assign (segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 120 and name CB)	14.06	0.96	0.96
20	assign (segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 121 and name CA)	11.08	0.46	0.45
	assign (segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 121 and name CB)	11.51	0.37	0.38
	assign (segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 122 and name CA)	12.30	0.50	0.50
	assign (segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 122 and name CB)	13.80	0.51	0.50
	assign (segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 123 and name CA)	11.66	0.66	0.67
25	assign (segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 123 and name CB)	12.56	0.86	0.86
	assign (segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 124 and name CA)	8.39	0.94	0.94
	assign (segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 124 and name CB)	8.30	1.28	1.29
	assign (segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 125 and name CA)	7.25	0.76	0.77
	assign (segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 125 and name CB)	7.54	1.12	1.11
30	assign (segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 126 and name CA)	9.69	0.79	0.78
	assign (segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 127 and name CA)	9.88	0.91	0.91
	assign (segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 127 and name CB)	10.17	1.54	1.54
	assign (segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 128 and name CA)	7.72	0.83	0.83
	assign (segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 128 and name CB)	6.88	0.88	0.88
35	assign (segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 129 and name CA)	8.00	1.32	1.32
	assign (segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 129 and name CB)	7.98	1.83	1.82
	assign (segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 130 and name CA)	11.02	0.75	0.75
	assign (segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 130 and name CB)	11.71	0.57	0.57
	assign (segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 131 and name CA)	11.38	0.61	0.62
40	assign (segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 131 and name CB)	11.08	1.16	1.15
	assign (segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 132 and name CA)	10.50	0.51	0.50
	assign (segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 132 and name CB)	9.51	0.84	0.84
	assign (segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 133 and name CA)	12.36	1.44	1.44
	assign (segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 133 and name CB)	12.35	1.79	1.79
45	assign (segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 134 and name CA)	14.76	0.60	0.60
	assign (segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 135 and name CA)	14.91	0.48	0.47
	assign (segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 135 and name CB)	14.08	0.64	0.64
	assign (segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 136 and name CA)	15.38	0.85	0.85
	assign (segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 136 and name CB)	14.56	1.21	1.21
50	assign (segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 137 and name CA)	17.71	1.00	1.01
	assign (segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 140 and name CA)	17.89	1.07	1.07
	assign (segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 141 and name CA)	16.25	1.88	1.89
	assign (segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 141 and name CB)	16.77	2.63	2.63
	assign (segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 255 and name CA)	17.93	0.87	0.87
55	assign (segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 256 and name CA)	15.69	0.91	0.91
	assign (segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 257 and name CA)	17.19	0.84	0.85
	assign (segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 258 and name CA)	17.99	0.59	0.59
	assign (segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 258 and name CB)	18.91	0.61	0.61
	assign (segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 259 and name CA)	14.70	0.71	0.71
60	assign (segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 259 and name CB)	14.03	0.76	0.75
	assign (segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 260 and name CA)	13.11	0.62	0.61
	assign (segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 260 and name CB)	13.29	0.79	0.79
	assign (segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 261 and name CA)	16.14	0.51	0.52
	assign (segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 262 and name CA)	16.10	0.74	0.74
65	assign (segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 262 and name CB)	16.24	0.88	0.88
	assign (segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 263 and name CA)	12.76	0.69	0.69
	assign (segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 263 and name CB)	11.39	0.68	0.69
	assign (segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 264 and name CA)	14.06	0.56	0.57
	assign (segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 265 and name CA)	17.43	0.61	0.61
70	assign (segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 266 and name CA)	16.30	0.66	0.65
	assign (segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 267 and name CA)	14.79	0.45	0.46
	assign (segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 267 and name CB)	13.59	0.43	0.43
	assign (segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 268 and name CA)	18.00	0.44	0.43
	assign (segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 268 and name CB)	18.61	0.41	0.41
75	assign (segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 270 and name CB)	17.39	0.59	0.59
	assign (segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 280 and name CB)	18.59	0.65	0.64
	assign (segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 281 and name CA)	18.64	0.63	0.63
	assign (segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 281 and name CB)	18.69	0.63	0.63
	assign (segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 305 and name CB)	17.32	0.99	0.98
80	assign (segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 309 and name CB)	17.93	1.10	1.10
	assign (segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 396 and name CA)	17.14	1.16	1.17
	assign (segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 396 and name CB)	17.23	1.16	1.15

5	assign	(segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 397 and name CA)	16.32	0.93	0.93
	assign	(segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 397 and name CB)	17.37	0.87	0.87
	assign	(segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 398 and name CA)	17.07	1.08	1.09
	assign	(segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 398 and name CB)	18.45	1.12	1.13
	assign	(segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 399 and name CA)	15.07	1.32	1.32
10	assign	(segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 399 and name CB)	15.38	1.40	1.40
	assign	(segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 400 and name CA)	11.87	1.11	1.11
	assign	(segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 400 and name CB)	11.88	1.00	1.00
	assign	(segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 401 and name CA)	12.80	0.96	0.95
	assign	(segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 402 and name CA)	13.88	1.18	1.17
15	assign	(segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 402 and name CB)	15.05	1.26	1.27
	assign	(segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 403 and name CA)	11.02	1.29	1.30
	assign	(segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 403 and name CB)	10.68	1.37	1.37
	assign	(segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 404 and name CA)	8.63	1.12	1.12
	assign	(segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 404 and name CB)	8.60	1.11	1.11
20	assign	(segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 405 and name CA)	11.42	1.16	1.16
	assign	(segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 405 and name CB)	12.74	1.15	1.14
	assign	(segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 406 and name CA)	12.47	1.12	1.12
	assign	(segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 407 and name CA)	9.48	0.99	0.99
	assign	(segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 407 and name CB)	8.33	1.07	1.08
25	assign	(segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 408 and name CA)	9.08	0.64	0.65
	assign	(segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 408 and name CB)	9.10	0.76	0.76
	assign	(segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 409 and name CA)	12.75	0.57	0.56
	assign	(segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 409 and name CB)	13.80	0.66	0.66
	assign	(segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 410 and name CA)	13.21	0.63	0.62
30	assign	(segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 411 and name CA)	11.29	0.36	0.36
	assign	(segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 411 and name CB)	9.87	0.33	0.34
	assign	(segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 412 and name CA)	12.65	0.66	0.65
	assign	(segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 413 and name CA)	16.66	1.08	1.08
	assign	(segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 414 and name CA)	16.00	0.99	1.00
35	assign	(segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 415 and name CA)	18.28	0.53	0.53
	assign	(segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 438 and name CA)	16.89	0.83	0.83
	assign	(segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 439 and name CA)	16.61	0.76	0.75
	assign	(segid 3A4 and resid 105 and name CA)	(segid 3A4 and resid 440 and name CA)	15.43	0.66	0.65
	assign	(segid 3A4 and resid 105 and name CB)	(segid 3A4 and resid 106 and name C)	5.39	0.08	0.07
40	assign	(segid 3A4 and resid 105 and name CB)	(segid 3A4 and resid 106 and name CA)	4.44	0.08	0.08
	assign	(segid 3A4 and resid 105 and name CB)	(segid 3A4 and resid 106 and name CB)	5.30	0.10	0.11
	assign	(segid 3A4 and resid 105 and name CB)	(segid 3A4 and resid 106 and name N)	3.14	0.08	0.08
	assign	(segid 3A4 and resid 105 and name CB)	(segid 3A4 and resid 106 and name O)	6.20	0.10	0.09
	assign	(segid 3A4 and resid 105 and name CB)	(segid 3A4 and resid 107 and name C)	6.93	0.09	0.09
45	assign	(segid 3A4 and resid 105 and name CB)	(segid 3A4 and resid 107 and name CA)	6.79	0.06	0.07
	assign	(segid 3A4 and resid 105 and name CB)	(segid 3A4 and resid 107 and name CB)	7.28	0.09	0.09
	assign	(segid 3A4 and resid 105 and name CB)	(segid 3A4 and resid 107 and name N)	5.59	0.05	0.06
	assign	(segid 3A4 and resid 105 and name CB)	(segid 3A4 and resid 108 and name C)	6.98	0.08	0.09
	assign	(segid 3A4 and resid 105 and name CB)	(segid 3A4 and resid 108 and name CA)	6.56	0.16	0.17
50	assign	(segid 3A4 and resid 105 and name CB)	(segid 3A4 and resid 108 and name CB)	5.85	0.30	0.30
	assign	(segid 3A4 and resid 105 and name CB)	(segid 3A4 and resid 108 and name N)	6.08	0.14	0.14
	assign	(segid 3A4 and resid 105 and name CB)	(segid 3A4 and resid 109 and name CA)	7.15	0.18	0.17
	assign	(segid 3A4 and resid 105 and name CB)	(segid 3A4 and resid 109 and name CB)	6.53	0.21	0.20
	assign	(segid 3A4 and resid 105 and name CB)	(segid 3A4 and resid 109 and name N)	6.36	0.12	0.13
55	assign					

	assign (segid 3A4 and resid 105 and name CB) (segid 3A4 and resid 133 and name CB)	11.48	1.71	1.70
	assign (segid 3A4 and resid 105 and name CB) (segid 3A4 and resid 134 and name CA)	14.05	0.43	0.42
	assign (segid 3A4 and resid 105 and name CB) (segid 3A4 and resid 135 and name CA)	14.38	0.40	0.41
	assign (segid 3A4 and resid 105 and name CB) (segid 3A4 and resid 135 and name CB)	13.62	0.65	0.65
5	assign (segid 3A4 and resid 105 and name CB) (segid 3A4 and resid 136 and name CA)	14.83	0.73	0.74
	assign (segid 3A4 and resid 105 and name CB) (segid 3A4 and resid 136 and name CB)	13.99	1.05	1.06
	assign (segid 3A4 and resid 105 and name CB) (segid 3A4 and resid 137 and name CA)	17.05	0.89	0.89
	assign (segid 3A4 and resid 105 and name CB) (segid 3A4 and resid 138 and name CA)	19.01	0.41	0.41
	assign (segid 3A4 and resid 105 and name CB) (segid 3A4 and resid 139 and name CA)	18.64	0.58	0.57
10	assign (segid 3A4 and resid 105 and name CB) (segid 3A4 and resid 140 and name CA)	17.66	0.95	0.96
	assign (segid 3A4 and resid 105 and name CB) (segid 3A4 and resid 140 and name CB)	17.66	0.86	0.85
	assign (segid 3A4 and resid 105 and name CB) (segid 3A4 and resid 141 and name CA)	16.24	1.84	1.84
	assign (segid 3A4 and resid 105 and name CB) (segid 3A4 and resid 255 and name CA)	16.80	0.65	0.65
	assign (segid 3A4 and resid 105 and name CB) (segid 3A4 and resid 256 and name CA)	14.64	0.66	0.66
15	assign (segid 3A4 and resid 105 and name CB) (segid 3A4 and resid 257 and name CA)	16.12	0.78	0.77
	assign (segid 3A4 and resid 105 and name CB) (segid 3A4 and resid 258 and name CA)	16.77	0.45	0.45
	assign (segid 3A4 and resid 105 and name CB) (segid 3A4 and resid 258 and name CB)	17.66	0.45	0.46
	assign (segid 3A4 and resid 105 and name CB) (segid 3A4 and resid 259 and name CA)	13.44	0.53	0.52
	assign (segid 3A4 and resid 105 and name CB) (segid 3A4 and resid 259 and name CB)	12.76	0.53	0.54
20	assign (segid 3A4 and resid 105 and name CB) (segid 3A4 and resid 260 and name CA)	11.97	0.68	0.67
	assign (segid 3A4 and resid 105 and name CB) (segid 3A4 and resid 260 and name CB)	12.23	0.90	0.91
	assign (segid 3A4 and resid 105 and name CB) (segid 3A4 and resid 261 and name CA)	15.02	0.55	0.55
	assign (segid 3A4 and resid 105 and name CB) (segid 3A4 and resid 262 and name CA)	14.86	0.64	0.64
	assign (segid 3A4 and resid 105 and name CB) (segid 3A4 and resid 262 and name CB)	14.95	0.75	0.75
25	assign (segid 3A4 and resid 105 and name CB) (segid 3A4 and resid 263 and name CA)	11.59	0.64	0.63
	assign (segid 3A4 and resid 105 and name CB) (segid 3A4 and resid 263 and name CB)	10.21	0.61	0.62
	assign (segid 3A4 and resid 105 and name CB) (segid 3A4 and resid 264 and name CA)	13.10	0.61	0.61
	assign (segid 3A4 and resid 105 and name CB) (segid 3A4 and resid 265 and name CA)	16.39	0.64	0.63
	assign (segid 3A4 and resid 105 and name CB) (segid 3A4 and resid 266 and name CA)	15.23	0.69	0.69
30	assign (segid 3A4 and resid 105 and name CB) (segid 3A4 and resid 267 and name CA)	13.96	0.53	0.52
	assign (segid 3A4 and resid 105 and name CB) (segid 3A4 and resid 267 and name CB)	12.80	0.51	0.51
	assign (segid 3A4 and resid 105 and name CB) (segid 3A4 and resid 268 and name CA)	17.21	0.51	0.51
	assign (segid 3A4 and resid 105 and name CB) (segid 3A4 and resid 268 and name CB)	17.79	0.49	0.49
	assign (segid 3A4 and resid 105 and name CB) (segid 3A4 and resid 270 and name CA)	17.89	0.67	0.67
35	assign (segid 3A4 and resid 105 and name CB) (segid 3A4 and resid 270 and name CB)	16.62	0.70	0.69
	assign (segid 3A4 and resid 105 and name CB) (segid 3A4 and resid 271 and name CB)	17.89	0.79	0.79
	assign (segid 3A4 and resid 105 and name CB) (segid 3A4 and resid 280 and name CB)	17.81	0.92	0.93
	assign (segid 3A4 and resid 105 and name CB) (segid 3A4 and resid 281 and name CA)	18.14	0.98	0.98
	assign (segid 3A4 and resid 105 and name CB) (segid 3A4 and resid 281 and name CB)	18.27	0.95	0.95
40	assign (segid 3A4 and resid 105 and name CB) (segid 3A4 and resid 305 and name CA)	17.50	1.14	1.14
	assign (segid 3A4 and resid 105 and name CB) (segid 3A4 and resid 305 and name CB)	16.33	1.17	1.17
	assign (segid 3A4 and resid 105 and name CB) (segid 3A4 and resid 309 and name CA)	17.42	1.11	1.10
	assign (segid 3A4 and resid 105 and name CB) (segid 3A4 and resid 309 and name CB)	16.68	1.19	1.19
	assign (segid 3A4 and resid 105 and name CB) (segid 3A4 and resid 312 and name CB)	18.03	0.99	0.99
45	assign (segid 3A4 and resid 105 and name CB) (segid 3A4 and resid 396 and name CA)	15.94	1.01	1.01
	assign (segid 3A4 and resid 105 and name CB) (segid 3A4 and resid 396 and name CB)	16.06	0.96	0.96
	assign (segid 3A4 and resid 105 and name CB) (segid 3A4 and resid 397 and name CA)	15.02	0.79	0.78
	assign (segid 3A4 and resid 105 and name CB) (segid 3A4 and resid 397 and name CB)	16.05	0.74	0.73
	assign (segid 3A4 and resid 105 and name CB) (segid 3A4 and resid 398 and name CA)	15.77	1.06	1.06
50	assign (segid 3A4 and resid 105 and name CB) (segid 3A4 and resid 398 and name CB)	17.16	1.11	1.11
	assign (segid 3A4 and resid 105 and name CB) (segid 3A4 and resid 399 and name CA)	13.87	1.33	1.33
	assign (segid 3A4 and resid 105 and name CB) (segid 3A4 and resid 399 and name CB)	14.22	1.39	1.39
	assign (segid 3A4 and resid 105 and name CB) (segid 3A4 and resid 400 and name CA)	10.63	1.04	1.05
	assign (segid 3A4 and resid 105 and name CB) (segid 3A4 and resid 400 and name CB)	10.64	0.85	0.85
55	assign (segid 3A4 and resid 105 and name CB) (segid 3A4 and resid 401 and name CA)	11.51	0.98	0.97
	assign (segid 3A4 and resid 105 and name CB) (segid 3A4 and resid 402 and name CA)	12.71	1.33	1.32
	assign (segid 3A4 and resid 105 and name CB) (segid 3A4 and resid 402 and name CB)	13.69	1.42	1.42
	assign (segid 3A4 and resid 105 and name CB) (segid 3A4 and resid 403 and name CA)	9.98	1.49	1.49
	assign (segid 3A4 and resid 105 and name CB) (segid 3A4 and resid 403 and name CB)	9.65	1.53	1.53
60	assign (segid 3A4 and resid 105 and name CB) (segid 3A4 and resid 404 and name CA)	7.56	1.26	1.26
	assign (segid 3A4 and resid 105 and name CB) (segid 3A4 and resid 404 and name CB)	7.44	1.18	1.18
	assign (segid 3A4 and resid 105 and name CB) (segid 3A4 and resid 405 and name CA)	10.46	1.36	1.37
	assign (segid 3A4 and resid 105 and name CB) (segid 3A4 and resid 405 and name CB)	11.72	1.34	1.33
	assign (segid 3A4 and resid 105 and name CB) (segid 3A4 and resid 406 and name CA)	11.70	1.42	1.42
65	assign (segid 3A4 and resid 105 and name CB) (segid 3A4 and resid 407 and name CA)	9.01	1.29	1.28
	assign (segid 3A4 and resid 105 and name CB) (segid 3A4 and resid 407 and name CB)	7.86	1.35	1.35
	assign (segid 3A4 and resid 105 and name CB) (segid 3A4 and resid 408 and name CA)	8.70	0.84	0.84
	assign (segid 3A4 and resid 105 and name CB) (segid 3A4 and resid 408 and name CB)	8.59	0.91	0.90
	assign (segid 3A4 and resid 105 and name CB) (segid 3A4 and resid 409 and name CA)	12.37	0.85	0.84
70	assign (segid 3A4 and resid 105 and name CB) (segid 3A4 and resid 409 and name CB)	13.31	0.95	0.95
	assign (segid 3A4 and resid 105 and name CB) (segid 3A4 and resid 410 and name CA)	13.05	0.98	0.98
	assign (segid 3A4 and resid 105 and name CB) (segid 3A4 and resid 411 and name CA)	11.49	0.58	0.59
	assign (segid 3A4 and resid 105 and name CB) (segid 3A4 and resid 411 and name CB)	10.14	0.53	0.53
	assign (segid 3A4 and resid 105 and name CB) (segid 3A4 and resid 412 and name CA)	12.77	0.70	0.69
75	assign (segid 3A4 and resid 105 and name CB) (segid 3A4 and resid 413 and name CA)	16.64	1.13	1.13
	assign (segid 3A4 and resid 105 and name CB) (segid 3A4 and resid 414 and name CA)	15.85	1.06	1.07
	assign (segid 3A4 and resid 105 and name CB) (segid 3A4 and resid 415 and name CA)	18.09	0.52	0.52
	assign (segid 3A4 and resid 105 and name CB) (segid 3A4 and resid 416 and name CA)	19.07	0.56	0.56
	assign (segid 3A4 and resid 105 and name CB) (segid 3A4 and resid 435 and name CA)	18.50	0.71	0.71
80	assign (segid 3A4 and resid 105 and name CB) (segid 3A4 and resid 437 and name CA)	17.64	1.17	1.18
	assign (segid 3A4 and resid 105 and name CB) (segid 3A4 and resid 438 and name CA)	16.43	0.98	0.98
	assign (segid 3A4 and resid 105 and name CB) (segid 3A4 and resid 439 and name CA)	16.42	0.92	0.93
	assign (segid 3A4 and resid 105 and name CB) (segid 3A4 and resid 440 and name CA)	15.33	0.75	0.75

	assign	(segid 3A4 and resid 105 and name N)	(segid 3A4 and resid 105 and name C)	2.46	0.02	0.01
	assign	(segid 3A4 and resid 105 and name N)	(segid 3A4 and resid 105 and name CA)	1.46	0.01	0.00
	assign	(segid 3A4 and resid 105 and name N)	(segid 3A4 and resid 105 and name CB)	2.44	0.03	0.04
	assign	(segid 3A4 and resid 105 and name N)	(segid 3A4 and resid 105 and name O)	3.49	0.04	0.04
5	assign	(segid 3A4 and resid 105 and name N)	(segid 3A4 and resid 106 and name C)	4.67	0.02	0.03
	assign	(segid 3A4 and resid 105 and name N)	(segid 3A4 and resid 106 and name CA)	4.21	0.03	0.02
	assign	(segid 3A4 and resid 105 and name N)	(segid 3A4 and resid 106 and name CB)	4.98	0.05	0.04
	assign	(segid 3A4 and resid 105 and name N)	(segid 3A4 and resid 106 and name N)	2.80	0.04	0.03
	assign	(segid 3A4 and resid 105 and name N)	(segid 3A4 and resid 106 and name O)	5.71	0.04	0.04
10	assign	(segid 3A4 and resid 105 and name N)	(segid 3A4 and resid 107 and name C)	5.63	0.09	0.08
	assign	(segid 3A4 and resid 105 and name N)	(segid 3A4 and resid 107 and name CA)	5.29	0.04	0.04
	assign	(segid 3A4 and resid 105 and name N)	(segid 3A4 and resid 107 and name CB)	5.36	0.08	0.07
	assign	(segid 3A4 and resid 105 and name N)	(segid 3A4 and resid 107 and name N)	4.29	0.03	0.03
	assign	(segid 3A4 and resid 105 and name N)	(segid 3A4 and resid 107 and name O)	6.83	0.09	0.09
15	assign	(segid 3A4 and resid 105 and name N)	(segid 3A4 and resid 108 and name C)	6.52	0.07	0.06
	assign	(segid 3A4 and resid 105 and name N)	(segid 3A4 and resid 108 and name CA)	5.66	0.11	0.11
	assign	(segid 3A4 and resid 105 and name N)	(segid 3A4 and resid 108 and name CB)	5.11	0.18	0.17
	assign	(segid 3A4 and resid 105 and name N)	(segid 3A4 and resid 108 and name N)	4.86	0.10	0.10
	assign	(segid 3A4 and resid 105 and name N)	(segid 3A4 and resid 108 and name O)	1.69	0.08	0.09
20	assign	(segid 3A4 and resid 105 and name N)	(segid 3A4 and resid 109 and name CA)	7.34	0.15	0.14
	assign	(segid 3A4 and resid 105 and name N)	(segid 3A4 and resid 109 and name CB)	7.11	0.18	0.19
	assign	(segid 3A4 and resid 105 and name N)	(segid 3A4 and resid 109 and name N)	6.20	0.09	0.10
	assign	(segid 3A4 and resid 105 and name N)	(segid 3A4 and resid 109 and name CB)	3.29	0.09	0.09
	assign	(segid 3A4 and resid 105 and name O)	(segid 3A4 and resid 106 and name C)	2.96	0.07	0.07
25	assign	(segid 3A4 and resid 105 and name O)	(segid 3A4 and resid 106 and name CA)	2.76	0.04	0.04
	assign	(segid 3A4 and resid 105 and name O)	(segid 3A4 and resid 106 and name CB)	4.26	0.04	0.04
	assign	(segid 3A4 and resid 105 and name O)	(segid 3A4 and resid 106 and name N)	2.26	0.02	0.01
	assign	(segid 3A4 and resid 105 and name O)	(segid 3A4 and resid 106 and name O)	3.34	0.10	0.09
	assign	(segid 3A4 and resid 105 and name O)	(segid 3A4 and resid 107 and name C)	4.19	0.13	0.13
30	assign	(segid 3A4 and resid 105 and name O)	(segid 3A4 and resid 107 and name CA)	4.43	0.11	0.11
	assign	(segid 3A4 and resid 105 and name O)	(segid 3A4 and resid 107 and name CB)	5.41	0.12	0.12
	assign	(segid 3A4 and resid 105 and name O)	(segid 3A4 and resid 107 and name N)	3.48	0.08	0.08
	assign	(segid 3A4 and resid 105 and name O)	(segid 3A4 and resid 107 and name O)	5.07	0.16	0.16
	assign	(segid 3A4 and resid 105 and name O)	(segid 3A4 and resid 108 and name C)	3.94	0.09	0.08
35	assign	(segid 3A4 and resid 105 and name O)	(segid 3A4 and resid 108 and name CA)	3.87	0.16	0.15
	assign	(segid 3A4 and resid 105 and name O)	(segid 3A4 and resid 108 and name CB)	3.71	0.26	0.26
	assign	(segid 3A4 and resid 105 and name O)	(segid 3A4 and resid 108 and name N)	3.44	0.17	0.16
	assign	(segid 3A4 and resid 105 and name O)	(segid 3A4 and resid 108 and name O)	5.09	0.10	0.10
	assign	(segid 3A4 and resid 105 and name O)	(segid 3A4 and resid 109 and name C)	5.14	0.13	0.14
40	assign	(segid 3A4 and resid 105 and name O)	(segid 3A4 and resid 109 and name CA)	4.00	0.15	0.16
	assign	(segid 3A4 and resid 105 and name O)	(segid 3A4 and resid 109 and name CB)	3.64	0.18	0.19
	assign	(segid 3A4 and resid 105 and name O)	(segid 3A4 and resid 109 and name N)	3.15	0.09	0.09
	assign	(segid 3A4 and resid 105 and name O)	(segid 3A4 and resid 109 and name O)	6.26	0.13	0.14
	assign	(segid 3A4 and resid 105 and name O)	(segid 3A4 and resid 110 and name C)	7.46	0.16	0.16
45	assign	(segid 3A4 and resid 105 and name O)	(segid 3A4 and resid 110 and name CA)	6.50	0.11	0.12
	assign	(segid 3A4 and resid 105 and name O)	(segid 3A4 and resid 110 and name CB)	6.72	0.10	0.10
	assign	(segid 3A4 and resid 105 and name O)	(segid 3A4 and resid 110 and name N)	5.17	0.12	0.12
	assign	(segid 3A4 and resid 105 and name O)	(segid 3A4 and resid 111 and name N)	7.21	0.2	

	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 108 and name N)	1.44	0.11	0.11
	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 108 and name O)	6.67	0.05	0.04
	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 109 and name C)	5.70	0.06	0.06
	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 109 and name CA)	5.17	0.09	0.09
	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 109 and name CB)	4.57	0.15	0.14
5	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 109 and name N)	4.58	0.06	0.06
	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 109 and name O)	6.85	0.10	0.09
	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 110 and name C)	7.44	0.05	0.05
	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 110 and name CA)	6.15	0.07	0.08
	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 110 and name CB)	5.87	0.08	0.08
10	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 110 and name N)	5.20	0.04	0.04
	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 111 and name CA)	8.89	0.20	0.21
	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 111 and name CB)	9.03	0.31	0.31
	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 111 and name N)	7.55	0.16	0.16
	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 112 and name CA)	10.40	0.14	0.14
15	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 119 and name CA)	12.71	1.59	1.58
	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 119 and name CB)	11.32	1.52	1.53
	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 119 and name N)	13.83	1.21	1.21
	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 120 and name CB)	14.77	1.18	1.18
	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 121 and name CA)	11.49	1.11	1.11
20	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 121 and name CB)	11.63	1.07	1.07
	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 122 and name CA)	13.65	1.05	1.05
	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 122 and name CB)	15.16	1.05	1.05
	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 123 and name CA)	13.53	0.86	0.85
	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 123 and name CB)	14.34	0.87	0.87
25	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 124 and name CA)	10.07	0.89	0.90
	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 124 and name CB)	9.54	1.05	1.05
	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 125 and name CA)	9.01	1.31	1.32
	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 125 and name CB)	8.73	1.85	1.84
	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 126 and name CA)	11.75	1.41	1.41
30	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 127 and name CA)	12.62	0.65	0.66
	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 127 and name CB)	12.89	1.16	1.16
	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 128 and name CA)	10.82	0.62	0.63
	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 128 and name CB)	9.90	0.70	0.70
	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 129 and name CA)	10.91	1.47	1.47
35	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 129 and name CB)	10.60	2.06	2.05
	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 130 and name CA)	13.99	0.97	0.97
	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 130 and name CB)	14.58	0.82	0.82
	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 131 and name CA)	14.61	0.36	0.37
	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 131 and name CB)	14.32	0.92	0.93
40	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 132 and name CA)	13.70	0.49	0.48
	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 132 and name CB)	12.67	0.77	0.77
	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 133 and name CA)	15.40	1.50	1.50
	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 133 and name CB)	15.30	1.91	1.91
45	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 134 and name CA)	17.90	0.52	0.53
	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 135 and name CA)	18.07	0.55	0.55
	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 135 and name CB)	17.25	0.79	0.78
	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 136 and name CA)	18.34	0.91	0.90
	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 136 and name CB)	17.43	1.24	1.24
50	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 256 and name CA)	18.54	0.55	0.55
	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 259 and name CA)	16.70	0.43	0.42
	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 259 and name CB)	16.16	0.37	0.37
	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 260 and name CA)	15.13	0.67	0.67
	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 260 and name CB)	15.52	0.79	0.79
55	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 261 and name CA)	17.73	0.72	0.72
	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 262 and name CA)	17.25	0.48	0.47
	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 262 and name CB)	17.45	0.35	0.34
	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 263 and name CA)	13.60	0.56	0.56
	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 263 and name CB)	12.44	0.55	0.55
60	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 264 and name CA)	14.74	0.79	0.78
	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 265 and name CA)	17.84	0.79	0.79
	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 266 and name CA)	16.19	0.79	0.79
	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 267 and name CA)	14.23	0.87	0.86
	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 267 and name CB)	13.10	0.93	0.93
65	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 268 and name CA)	17.54	0.96	0.95
	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 270 and name CA)	17.42	1.08	1.07
	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 270 and name CB)	16.08	1.04	1.04
	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 271 and name CB)	17.20	1.17	1.17
	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 277 and name CB)	17.14	1.27	1.27
	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 280 and name CA)	17.68	0.68	0.67
70	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 280 and name CB)	16.82	0.72	0.71
	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 281 and name CA)	16.20	0.76	0.75
	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 281 and name CB)	16.10	0.87	0.88
	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 305 and name CA)	17.52	0.68	0.69
	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 305 and name CB)	16.29	0.67	0.67
75	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 308 and name CB)	18.67	0.89	0.88
	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 309 and name CA)	18.64	0.69	0.68
	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 309 and name CB)	18.02	0.60	0.61
	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 396 and name CA)	18.97	0.58	0.58
	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 397 and name CA)	18.04	0.31	0.30
80	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 397 and name CB)	19.11	0.33	0.32
	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 398 and name CA)	18.11	0.38	0.39
	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 398 and name CB)	19.39	0.42	0.43

	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 399 and name CA)	16.07	0.60	0.60
	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 399 and name CB)	16.53	0.74	0.74
	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 400 and name CA)	13.26	0.37	0.38
	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 400 and name CB)	13.61	0.35	0.35
5	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 401 and name CA)	13.56	0.46	0.46
	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 402 and name CA)	13.90	0.43	0.43
	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 402 and name CB)	15.09	0.51	0.51
	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 403 and name CA)	11.05	0.52	0.52
	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 403 and name CB)	11.07	0.64	0.65
10	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 404 and name CA)	8.69	0.42	0.43
	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 404 and name CB)	9.07	0.50	0.50
	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 405 and name CA)	10.63	0.75	0.75
	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 405 and name CB)	12.06	0.75	0.76
	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 406 and name CA)	11.08	0.55	0.55
	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 407 and name CA)	7.65	0.50	0.51
15	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 407 and name CB)	6.83	0.54	0.54
	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 407 and name O)	6.85	0.64	0.63
	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 408 and name CA)	6.95	0.86	0.85
	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 408 and name CB)	7.37	1.07	1.08
20	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 409 and name CA)	10.31	0.72	0.72
	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 409 and name CB)	11.56	0.69	0.69
	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 410 and name CA)	10.35	0.47	0.48
	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 411 and name CA)	8.02	0.58	0.57
	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 411 and name CB)	6.59	0.58	0.59
25	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 412 and name CA)	9.56	1.12	1.12
	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 413 and name CA)	13.89	1.48	1.49
	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 414 and name CA)	13.82	1.27	1.27
	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 415 and name CA)	16.50	1.16	1.15
	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 438 and name CA)	17.09	1.46	1.45
30	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 439 and name CA)	16.33	1.23	1.23
	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 440 and name CA)	14.40	1.30	1.29
	assign (segid 3A4 and resid 106 and name CA)	(segid 3A4 and resid 107 and name C)	5.44	0.03	0.03
	assign (segid 3A4 and resid 106 and name CB)	(segid 3A4 and resid 107 and name CA)	4.48	0.05	0.04
	assign (segid 3A4 and resid 106 and name CB)	(segid 3A4 and resid 107 and name CB)	5.34	0.07	0.07
35	assign (segid 3A4 and resid 106 and name CB)	(segid 3A4 and resid 107 and name N)	3.15	0.05	0.05
	assign (segid 3A4 and resid 106 and name CB)	(segid 3A4 and resid 107 and name O)	6.26	0.09	0.09
	assign (segid 3A4 and resid 106 and name CB)	(segid 3A4 and resid 108 and name C)	6.93	0.05	0.05
	assign (segid 3A4 and resid 106 and name CB)	(segid 3A4 and resid 108 and name CA)	6.85	0.08	0.09
	assign (segid 3A4 and resid 106 and name CB)	(segid 3A4 and resid 108 and name CB)	7.31	0.18	0.18
40	assign (segid 3A4 and resid 106 and name CB)	(segid 3A4 and resid 108 and name N)	5.68	0.08	0.08
	assign (segid 3A4 and resid 106 and name CB)	(segid 3A4 and resid 109 and name C)	6.82	0.04	0.04
	assign (segid 3A4 and resid 106 and name CB)	(segid 3A4 and resid 109 and name CA)	6.49	0.07	0.08
	assign (segid 3A4 and resid 106 and name CB)	(segid 3A4 and resid 109 and name CB)	5.82	0.14	0.14
	assign (segid 3A4 and resid 106 and name CB)	(segid 3A4 and resid 109 and name N)	6.00	0.05	0.05
45	assign (segid 3A4 and resid 106 and name CB)	(segid 3A4 and resid 110 and name CA)	6.87	0.11	0.10
	assign (segid 3A4 and resid 106 and name CB)	(segid 3A4 and resid 110 and name CB)	6.33	0.12	0.13
	assign (segid 3A4 and resid 106 and name CB)	(segid 3A4 and resid 110 and name N)	6.16	0.05	0.05
	assign (segid 3A4 and resid 106 and name CB)	(segid 3A4 and resid 111 and name CA)	9.87	0.18	0.18
	assign (segid 3A4 and resid 106 and name CB)	(segid 3A4 and resid 111 and name CB)	10.05	0.27	0.28
50	assign (segid 3A4 and resid 106 and name CB)	(segid 3A4 and resid 112 and name CA)	11.54	0.13	0.14
	assign (segid 3A4 and resid 106 and name CB)	(segid 3A4 and resid 119 and name CA)	13.88	1.70	1.70
	assign (segid 3A4 and resid 106 and name CB)	(segid 3A4 and resid 119 and name CB)	12.50	1.65	1.65
	assign (segid 3A4 and resid 106 and name CB)	(segid 3A4 and resid 120 and name CA)	15.01	1.39	1.38
	assign (segid 3A4 and resid 106 and name CB)	(segid 3A4 and resid 120 and name CB)	16.00	1.33	1.33
55	assign (segid 3A4 and resid 106 and name CB)	(segid 3A4 and resid 121 and name CA)	12.51	1.36	1.35
	assign (segid 3A4 and resid 106 and name CB)	(segid 3A4 and resid 121 and name CB)	12.51	1.35	1.35
	assign (segid 3A4 and resid 106 and name CB)	(segid 3A4 and resid 122 and name CA)	14.68	1.24	1.24
	assign (segid 3A4 and resid 106 and name CB)	(segid 3A4 and resid 122 and name CB)	16.18	1.25	1.25
60	assign (segid 3A4 and resid 106 and name CB)	(segid 3A4 and resid 123 and name CA)	14.77	0.97	0.98
	assign (segid 3A4 and resid 106 and name CB)	(segid 3A4 and resid 123 and name CB)	15.63	0.95	0.95
	assign (segid 3A4 and resid 106 and name CB)	(segid 3A4 and resid 124 and name CA)	11.38	0.98	0.98
	assign (segid 3A4 and resid 106 and name CB)	(segid 3A4 and resid 124 and name CB)	10.86	1.12	1.12
	assign (segid 3A4 and resid 106 and name CB)	(segid 3A4 and resid 125 and name CA)	10.06	1.40	1.40
65	assign (segid 3A4 and resid 106 and name CB)	(segid 3A4 and resid 125 and name CB)	9.69	1.93	1.93
	assign (segid 3A4 and resid 106 and name CB)	(segid 3A4 and resid 126 and name CA)	12.61	1.58	1.57
	assign (segid 3A4 and resid 106 and name CB)	(segid 3A4 and resid 127 and name CA)	13.62	0.74	0.74
	assign (segid 3A4 and resid 106 and name CB)	(segid 3A4 and resid 127 and name CB)	13.97	1.17	1.18
	assign (segid 3A4 and resid 106 and name CB)	(segid 3A4 and resid 128 and name CA)	11.73	0.73	0.73
	assign (segid 3A4 and resid 106 and name CB)	(segid 3A4 and resid 128 and name CB)	10.86	0.84	0.84
70	assign (segid 3A4 and resid 106 and name CB)	(segid 3A4 and resid 129 and name CA)	11.51	1.46	1.47
	assign (segid 3A4 and resid 106 and name CB)	(segid 3A4 and resid 129 and name CB)	11.15	2.10	2.09
	assign (segid 3A4 and resid 106 and name CB)	(segid 3A4 and resid 130 and name CA)	14.53	1.09	1.09
	assign (segid 3A4 and resid 106 and name CB)	(segid 3A4 and resid 130 and name CB)	15.16	1.02	1.01
	assign (segid 3A4 and resid 106 and name CB)	(segid 3A4 and resid 131 and name CA)	15.26	0.37	0.36
75	assign (segid 3A4 and resid 106 and name CB)	(segid 3A4 and resid 131 and name CB)	15.05	0.96	0.96
	assign (segid 3A4 and resid 106 and name CB)	(segid 3A4 and resid 132 and name CA)	14.18	0.40	0.40
	assign (segid 3A4 and resid 106 and name CB)	(segid 3A4 and resid 132 and name CB)	13.16	0.65	0.64
	assign (segid 3A4 and resid 106 and name CB)	(segid 3A4 and resid 133 and name CA)	15.68	1.49	1.50
	assign (segid 3A4 and resid 106 and name CB)	(segid 3A4 and resid 133 and name CB)	15.55	1.96	1.95
80	assign (segid 3A4 and resid 106 and name CB)	(segid 3A4 and resid 134 and name CA)	18.27	0.47	0.47
	assign (segid 3A4 and resid 106 and name CB)	(segid 3A4 and resid 135 and name CA)	18.45	0.62	0.62
	assign (segid 3A4 and resid 106 and name CB)	(segid 3A4 and resid 135 and name CB)	17.67	0.92	0.92
	assign (segid 3A4 and resid 106 and name CB)	(segid 3A4 and resid 256 and name CA)	19.12	0.42	0.43

	assign (segid 3A4 and resid 106 and name O) (segid 3A4 and resid 108 and name CA)	4.28	0.13	0.12
	assign (segid 3A4 and resid 106 and name O) (segid 3A4 and resid 108 and name CB)	5.21	0.20	0.20
	assign (segid 3A4 and resid 106 and name O) (segid 3A4 and resid 108 and name N)	3.38	0.12	0.12
	assign (segid 3A4 and resid 106 and name O) (segid 3A4 and resid 108 and name O)	4.94	0.13	0.13
5	assign (segid 3A4 and resid 106 and name O) (segid 3A4 and resid 109 and name C)	3.65	0.06	0.05
	assign (segid 3A4 and resid 106 and name O) (segid 3A4 and resid 109 and name CA)	3.58	0.05	0.05
	assign (segid 3A4 and resid 106 and name O) (segid 3A4 and resid 109 and name CB)	3.52	0.08	0.07
	assign (segid 3A4 and resid 106 and name O) (segid 3A4 and resid 109 and name N)	3.09	0.08	0.08
	assign (segid 3A4 and resid 106 and name O) (segid 3A4 and resid 109 and name O)	4.81	0.06	0.06
10	assign (segid 3A4 and resid 106 and name O) (segid 3A4 and resid 110 and name C)	5.06	0.06	0.07
	assign (segid 3A4 and resid 106 and name O) (segid 3A4 and resid 110 and name CA)	3.81	0.07	0.07
	assign (segid 3A4 and resid 106 and name O) (segid 3A4 and resid 110 and name CB)	3.63	0.06	0.05
	assign (segid 3A4 and resid 106 and name O) (segid 3A4 and resid 110 and name N)	2.90	0.05	0.06
	assign (segid 3A4 and resid 106 and name O) (segid 3A4 and resid 110 and name O)	6.13	0.06	0.05
15	assign (segid 3A4 and resid 106 and name O) (segid 3A4 and resid 111 and name C)	7.45	0.14	0.15
	assign (segid 3A4 and resid 106 and name O) (segid 3A4 and resid 111 and name CA)	6.60	0.18	0.19
	assign (segid 3A4 and resid 106 and name O) (segid 3A4 and resid 111 and name CB)	6.88	0.25	0.26
	assign (segid 3A4 and resid 106 and name O) (segid 3A4 and resid 111 and name N)	5.21	0.15	0.16
	assign (segid 3A4 and resid 106 and name O) (segid 3A4 and resid 112 and name N)	7.18	0.12	0.11
20	assign (segid 3A4 and resid 106 and name O) (segid 3A4 and resid 411 and name CB)	6.59	0.53	0.53
	assign (segid 3A4 and resid 107 and name C) (segid 3A4 and resid 107 and name CB)	2.47	0.03	0.04
	assign (segid 3A4 and resid 107 and name C) (segid 3A4 and resid 107 and name O)	1.23	0.01	0.01
	assign (segid 3A4 and resid 107 and name C) (segid 3A4 and resid 108 and name C)	3.00	0.05	0.05
	assign (segid 3A4 and resid 107 and name C) (segid 3A4 and resid 108 and name CA)	2.43	0.02	0.02
25	assign (segid 3A4 and resid 107 and name C) (segid 3A4 and resid 108 and name CB)	3.68	0.02	0.02
	assign (segid 3A4 and resid 107 and name C) (segid 3A4 and resid 108 and name N)	1.32	0.01	0.01
	assign (segid 3A4 and resid 107 and name C) (segid 3A4 and resid 108 and name O)	3.88	0.13	0.13
	assign (segid 3A4 and resid 107 and name C) (segid 3A4 and resid 109 and name C)	4.46	0.09	0.10
30	assign (segid 3A4 and resid 107 and name C) (segid 3A4 and resid 109 and name CA)	4.41	0.07	0.07
	assign (segid 3A4 and resid 107 and name C) (segid 3A4 and resid 109 and name CB)	5.20	0.12	0.11
	assign (segid 3A4 and resid 107 and name C) (segid 3A4 and resid 109 and name N)	3.22	0.08	0.08
	assign (segid 3A4 and resid 107 and name C) (segid 3A4 and resid 109 and name O)	5.55	0.12	0.11
	assign (segid 3A4 and resid 107 and name C) (segid 3A4 and resid 110 and name C)	4.94	0.30	0.30
35	assign (segid 3A4 and resid 107 and name C) (segid 3A4 and resid 110 and name CA)	4.41	0.15	0.16
	assign (segid 3A4 and resid 107 and name C) (segid 3A4 and resid 110 and name CB)	4.11	0.17	0.17
	assign (segid 3A4 and resid 107 and name C) (segid 3A4 and resid 110 and name N)	3.70	0.17	0.16
	assign (segid 3A4 and resid 107 and name C) (segid 3A4 and resid 110 and name O)	6.11	0.31	0.32
	assign (segid 3A4 and resid 107 and name C) (segid 3A4 and resid 111 and name C)	6.51	0.43	0.43
40	assign (segid 3A4 and resid 107 and name C) (segid 3A4 and resid 111 and name CA)	5.41	0.48	0.49
	assign (segid 3A4 and resid 107 and name C) (segid 3A4 and resid 111 and name CB)	5.08	0.54	0.53
	assign (segid 3A4 and resid 107 and name C) (segid 3A4 and resid 111 and name N)	4.40	0.40	0.41
	assign (segid 3A4 and resid 107 and name C) (segid 3A4 and resid 112 and name N)	6.66	0.30	0.29
	assign (segid 3A4 and resid 107 and name CA) (segid 3A4 and resid 107 and name C)	1.50	0.01	0.02
45	assign (segid 3A4 and resid 107 and name CA) (segid 3A4 and resid 107 and name CB)	1.51	0.02	0.02
	assign (segid 3A4 and resid 107 and name CA) (segid 3A4 and resid 107 and name O)	2.38	0.04	0.03
	assign (segid 3A4 and resid 107 and name CA) (segid 3A4 and resid 108 and name C)	4.37	0.04	0.04
	assign (segid 3A4 and resid 107 and name CA) (segid 3A4 and resid 108 and name CA)	3.78	0.01	0.01
	assign (segid 3A4 and resid 107 and name CA) (segid 3A4 and resid 108 and name CB)	4.80	0.06	0.06
50	assign (segid 3A4 and resid 107 and name CA) (segid 3A4 and resid 108 and name N)	2.41	0.02	0.02
	assign (segid 3A4 and resid 107 and name CA) (segid 3A4 and resid 108 and name O)	5.32	0.12	0.12
	assign (segid 3A4 and resid 107 and name CA) (segid 3A4 and resid 109 and name C)	5.38	0.06	0.05
	assign (segid 3A4 and resid 107 and name CA) (segid 3A4 and resid 109 and name CA)	5.38	0.05	0.04
	assign (segid 3A4 and resid 107 and name CA) (segid 3A4 and resid 109 and name CB)	5.85	0.11	0.10
55	assign (segid 3A4 and resid 107 and name CA) (segid 3A4 and resid 109 and name N)	4.29	0.06	0.06
	assign (segid 3A4 and resid 107 and name CA) (segid 3A4 and resid 109 and name O)	6.50	0.07	0.08
	assign (segid 3A4 and resid 107 and name CA) (segid 3A4 and resid 110 and name C)	5.73	0.24	0.24
	assign (segid 3A4 and resid 107 and name CA) (segid 3A4 and resid 110 and name CA)	4.96	0.09	0.08
	assign (segid 3A4 and resid 107 and name CA) (segid 3A4 and resid 110 and name CB)	4.25	0.11	0.11
60	assign (segid 3A4 and resid 107 and name CA) (segid 3A4 and resid 110 and name N)	4.42	0.09	0.10
	assign (segid 3A4 and resid 107 and name CA) (segid 3A4 and resid 110 and name O)	6.83	0.26	0.26
	assign (segid 3A4 and resid 107 and name CA) (segid 3A4 and resid 111 and name CA)	6.54	0.42	0.41
	assign (segid 3A4 and resid 107 and name CA) (segid 3A4 and resid 111 and name CB)	6.28	0.47	0.47
	assign (segid 3A4 and resid 107 and name CA) (segid 3A4 and resid 111 and name N)	5.44	0.33	0.32
	assign (segid 3A4 and resid 107 and name CA) (segid 3A4 and resid 112 and name CA)	9.17	0.18	0.19
65	assign (segid 3A4 and resid 107 and name CA) (segid 3A4 and resid 119 and name CA)	13.48	0.97	0.98
	assign (segid 3A4 and resid 107 and name CA) (segid 3A4 and resid 119 and name CB)	12.15	0.87	0.87
	assign (segid 3A4 and resid 107 and name CA) (segid 3A4 and resid 120 and name CA)	15.11	0.50	0.50
	assign (segid 3A4 and resid 107 and name CA) (segid 3A4 and resid 120 and name CB)	15.91	0.51	0.51
	assign (segid 3A4 and resid 107 and name CA) (segid 3A4 and resid 121 and name CA)	13.49	0.60	0.59
70	assign (segid 3A4 and resid 107 and name CA) (segid 3A4 and resid 121 and name CB)	13.90	0.65	0.65
	assign (segid 3A4 and resid 107 and name CA) (segid 3A4 and resid 122 and name CA)	15.66	0.75	0.76
	assign (segid 3A4 and resid 107 and name CA) (segid 3A4 and resid 122 and name CB)	17.15	0.73	0.74
	assign (segid 3A4 and resid 107 and name CA) (segid 3A4 and resid 123 and name CA)	14.79	0.51	0.51
	assign (segid 3A4 and resid 107 and name CA) (segid 3A4 and resid 123 and name CB)	15.36	0.59	0.58
75	assign (segid 3A4 and resid 107 and name CA) (segid 3A4 and resid 124 and name CA)	11.18	0.46	0.46
	assign (segid 3A4 and resid 107 and name CA) (segid 3A4 and resid 124 and name CB)	10.54	0.46	0.46
	assign (segid 3A4 and resid 107 and name CA) (segid 3A4 and resid 125 and name CA)	11.10	1.26	1.26
	assign (segid 3A4 and resid 107 and name CA) (segid 3A4 and resid 125 and name CB)	11.08	1.76	1.76
80	assign (segid 3A4 and resid 107 and name CA) (segid 3A4 and resid 126 and name CA)	14.03	1.10	1.10
	assign (segid 3A4 and resid 107 and name CA) (segid 3A4 and resid 127 and name CA)	14.25	0.92	0.92
	assign (segid 3A4 and resid 107 and name CA) (segid 3A4 and resid 127 and name CB)	14.27	1.46	1.47
	assign (segid 3A4 and resid 107 and name CA) (segid 3A4 and resid 128 and name CA)	12.31	0.84	0.85
	assign (segid 3A4 and resid 107 and name CA) (segid 3A4 and resid 128 and name CB)	11.35	0.78	0.77

	assign (segid 3A4 and resid 107 and name CA)	(segid 3A4 and resid 129 and name CA)	12.94	1.69	1.68
	assign (segid 3A4 and resid 107 and name CA)	(segid 3A4 and resid 129 and name CB)	12.92	2.11	2.12
	assign (segid 3A4 and resid 107 and name CA)	(segid 3A4 and resid 130 and name CA)	15.90	1.04	1.04
	assign (segid 3A4 and resid 107 and name CA)	(segid 3A4 and resid 130 and name CB)	16.53	0.84	0.83
5	assign (segid 3A4 and resid 107 and name CA)	(segid 3A4 and resid 131 and name CA)	15.94	1.20	1.20
	assign (segid 3A4 and resid 107 and name CA)	(segid 3A4 and resid 131 and name CB)	15.49	1.59	1.59
	assign (segid 3A4 and resid 107 and name CA)	(segid 3A4 and resid 132 and name CA)	14.91	1.33	1.33
	assign (segid 3A4 and resid 107 and name CA)	(segid 3A4 and resid 132 and name CB)	13.90	1.61	1.61
	assign (segid 3A4 and resid 107 and name CA)	(segid 3A4 and resid 133 and name CA)	16.94	1.82	1.82
10	assign (segid 3A4 and resid 107 and name CA)	(segid 3A4 and resid 259 and name CB)	18.96	0.74	0.75
	assign (segid 3A4 and resid 107 and name CA)	(segid 3A4 and resid 260 and name CA)	17.81	0.61	0.61
	assign (segid 3A4 and resid 107 and name CA)	(segid 3A4 and resid 260 and name CB)	17.98	0.75	0.76
	assign (segid 3A4 and resid 107 and name CA)	(segid 3A4 and resid 263 and name CA)	16.83	0.41	0.41
	assign (segid 3A4 and resid 107 and name CA)	(segid 3A4 and resid 263 and name CB)	15.61	0.44	0.45
15	assign (segid 3A4 and resid 107 and name CA)	(segid 3A4 and resid 264 and name CA)	17.67	0.38	0.38
	assign (segid 3A4 and resid 107 and name CA)	(segid 3A4 and resid 267 and name CA)	17.33	0.49	0.49
	assign (segid 3A4 and resid 107 and name CA)	(segid 3A4 and resid 267 and name CB)	16.12	0.49	0.49
	assign (segid 3A4 and resid 107 and name CA)	(segid 3A4 and resid 399 and name CA)	19.04	0.78	0.78
	assign (segid 3A4 and resid 107 and name CA)	(segid 3A4 and resid 400 and name CA)	16.22	0.66	0.67
20	assign (segid 3A4 and resid 107 and name CA)	(segid 3A4 and resid 400 and name CB)	16.47	0.69	0.70
	assign (segid 3A4 and resid 107 and name CA)	(segid 3A4 and resid 401 and name CA)	16.89	0.45	0.45
	assign (segid 3A4 and resid 107 and name CA)	(segid 3A4 and resid 402 and name CA)	17.21	0.46	0.46
	assign (segid 3A4 and resid 107 and name CA)	(segid 3A4 and resid 402 and name CB)	18.34	0.53	0.53
	assign (segid 3A4 and resid 107 and name CA)	(segid 3A4 and resid 403 and name CA)	14.13	0.54	0.54
25	assign (segid 3A4 and resid 107 and name CA)	(segid 3A4 and resid 403 and name CB)	13.99	0.69	0.68
	assign (segid 3A4 and resid 107 and name CA)	(segid 3A4 and resid 404 and name CA)	12.02	0.41	0.41
	assign (segid 3A4 and resid 107 and name CA)	(segid 3A4 and resid 404 and name CB)	12.39	0.46	0.47
	assign (segid 3A4 and resid 107 and name CA)	(segid 3A4 and resid 405 and name CA)	14.01	0.60	0.60
	assign (segid 3A4 and resid 107 and name CA)	(segid 3A4 and resid 405 and name CB)	15.47	0.59	0.59
30	assign (segid 3A4 and resid 107 and name CA)	(segid 3A4 and resid 406 and name CA)	14.16	0.56	0.57
	assign (segid 3A4 and resid 107 and name CA)	(segid 3A4 and resid 407 and name CA)	10.52	0.57	0.57
	assign (segid 3A4 and resid 107 and name CA)	(segid 3A4 and resid 407 and name CB)	9.68	0.51	0.50
	assign (segid 3A4 and resid 107 and name CA)	(segid 3A4 and resid 408 and name CA)	10.00	0.75	0.75
	assign (segid 3A4 and resid 107 and name CA)	(segid 3A4 and resid 408 and name CB)	10.57	0.84	0.85
35	assign (segid 3A4 and resid 107 and name CA)	(segid 3A4 and resid 409 and name CA)	13.03	0.84	0.84
	assign (segid 3A4 and resid 107 and name CA)	(segid 3A4 and resid 409 and name CB)	14.40	0.78	0.78
	assign (segid 3A4 and resid 107 and name CA)	(segid 3A4 and resid 410 and name CA)	12.49	0.96	0.96
	assign (segid 3A4 and resid 107 and name CA)	(segid 3A4 and resid 411 and name CA)	9.54	1.13	1.13
	assign (segid 3A4 and resid 107 and name CA)	(segid 3A4 and resid 411 and name CB)	8.12	1.11	1.11
40	assign (segid 3A4 and resid 107 and name CA)	(segid 3A4 and resid 412 and name CA)	11.27	1.32	1.31
	assign (segid 3A4 and resid 107 and name CA)	(segid 3A4 and resid 413 and name CA)	15.69	1.44	1.44
	assign (segid 3A4 and resid 107 and name CA)	(segid 3A4 and resid 414 and name CA)	15.87	1.17	1.16
	assign (segid 3A4 and resid 107 and name CA)	(segid 3A4 and resid 439 and name CA)	17.89	0.62	0.61
	assign (segid 3A4 and resid 107 and name CA)	(segid 3A4 and resid 440 and name CA)	16.03	0.86	0.85
45	assign (segid 3A4 and resid 107 and name CB)	(segid 3A4 and resid 108 and name C)	5.37	0.06	0.07
	assign (segid 3A4 and resid 107 and name CB)	(segid 3A4 and resid 108 and name CA)	4.43	0.08	0.09
	assign (segid 3A4 and resid 107 and name CB)	(segid 3A4 and resid 108 and name CB)	5.27	0.13	0.13
	assign (segid 3A4 and resid 107 and name CB)	(segid 3A4 and resid 108 and name N)	3.10	0.09	0.10
50	assign (segid 3A4 and resid 107 and name CB)	(segid 3A4 and resid 108 and name O)	6.27	0.12	0.13
	assign (segid 3A4 and resid 107 and name CB)	(segid 3A4 and resid 109 and name C)	6.77	0.06	0.06
	assign (segid 3A4 and resid 107 and name CB)	(segid 3A4 and resid 109 and name CA)	6.73	0.07	0.07
	assign (segid 3A4 and resid 107 and name CB)	(segid 3A4 and resid 109 and name CB)	7.27	0.12	0.12
	assign (segid 3A4 and resid 107 and name CB)	(segid 3A4 and resid 109 and name N)	5.53	0.09	0.10
	assign (segid 3A4 and resid 107 and name CB)	(segid 3A4 and resid 110 and name C)	6.84	0.27	0.26
55	assign (segid 3A4 and resid 107 and name CB)	(segid 3A4 and resid 110 and name CA)	6.25	0.09	0.09
	assign (segid 3A4 and resid 107 and name CB)	(segid 3A4 and resid 110 and name CB)	5.42	0.13	0.12
	assign (segid 3A4 and resid 107 and name CB)	(segid 3A4 and resid 110 and name N)	5.83	0.10	0.09
	assign (segid 3A4 and resid 107 and name CB)	(segid 3A4 and resid 111 and name CA)	7.30	0.47	0.48
	assign (segid 3A4 and resid 107 and name CB)	(segid 3A4 and resid 111 and name CB)	6.79	0.56	0.55
60	assign (segid 3A4 and resid 107 and name CB)	(segid 3A4 and resid 111 and name N)	6.41	0.36	0.35
	assign (segid 3A4 and resid 107 and name CB)	(segid 3A4 and resid 112 and name CA)	10.23	0.25	0.24
	assign (segid 3A4 and resid 107 and name CB)	(segid 3A4 and resid 119 and name CA)	14.73	0.86	0.87
	assign (segid 3A4 and resid 107 and name CB)	(segid 3A4 and resid 119 and name CB)	13.41	0.75	0.75
65	assign (segid 3A4 and resid 107 and name CB)	(segid 3A4 and resid 120 and name CA)	16.26	0.37	0.36
	assign (segid 3A4 and resid 107 and name CB)	(segid 3A4 and resid 120 and name CB)	16.99	0.46	0.45
	assign (segid 3A4 and resid 107 and name CB)	(segid 3A4 and resid 121 and name CA)	14.64	0.51	0.52
	assign (segid 3A4 and resid 107 and name CB)	(segid 3A4 and resid 121 and name CB)	15.10	0.59	0.60
	assign (segid 3A4 and resid 107 and name CB)	(segid 3A4 and resid 122 and name CA)	16.61	0.78	0.78
	assign (segid 3A4 and resid 107 and name CB)	(segid 3A4 and resid 122 and name CB)	18.09	0.77	0.78
70	assign (segid 3A4 and resid 107 and name CB)	(segid 3A4 and resid 123 and name CA)	15.56	0.66	0.66
	assign (segid 3A4 and resid 107 and name CB)	(segid 3A4 and resid 123 and name CB)	16.13	0.77	0.77
	assign (segid 3A4 and resid 107 and name CB)	(segid 3A4 and resid 124 and name CA)	11.99	0.56	0.55
	assign (segid 3A4 and resid 107 and name CB)	(segid 3A4 and resid 124 and name CB)	11.46	0.56	0.56
	assign (segid 3A4 and resid 107 and name CB)	(segid 3A4 and resid 125 and name CA)	11.90	1.22	1.21
75	assign (segid 3A4 and resid 107 and name CB)	(segid 3A4 and resid 125 and name CB)	12.00	1.66	1.66
	assign (segid 3A4 and resid 107 and name CB)	(segid 3A4 and resid 126 and name CA)	14.69	1.04	1.04
	assign (segid 3A4 and resid 107 and name CB)	(segid 3A4 and resid 127 and name CA)	14.67	1.21	1.20
	assign (segid 3A4 and resid 107 and name CB)	(segid 3A4 and resid 127 and name CB)	14.71	1.74	1.74
	assign (segid 3A4 and resid 107 and name CB)	(segid 3A4 and resid 128 and name CA)	12.54	1.10	1.11
80	assign (segid 3A4 and resid 107 and name CB)	(segid 3A4 and resid 128 and name CB)	11.63	1.00	1.00
	assign (segid 3A4 and resid 107 and name CB)	(segid 3A4 and resid 129 and name CA)	13.12	1.73	1.74
	assign (segid 3A4 and resid 107 and name CB)	(segid 3A4 and resid 129 and name CB)	13.23	2.09	2.10
	assign (segid 3A4 and resid 107 and name CB)	(segid 3A4 and resid 130 and name CA)	15.97	1.16	1.16

	assign (segid 3A4 and resid 107 and name CB)	(segid 3A4 and resid 130 and name CB)	16.66	1.00	1.00
	assign (segid 3A4 and resid 107 and name CB)	(segid 3A4 and resid 131 and name CA)	15.82	1.54	1.54
	assign (segid 3A4 and resid 107 and name CB)	(segid 3A4 and resid 131 and name CB)	15.40	1.95	1.94
	assign (segid 3A4 and resid 107 and name CB)	(segid 3A4 and resid 132 and name CA)	14.62	1.59	1.59
	assign (segid 3A4 and resid 107 and name CB)	(segid 3A4 and resid 132 and name CB)	13.65	1.85	1.84
5	assign (segid 3A4 and resid 107 and name CB)	(segid 3A4 and resid 133 and name CA)	16.64	1.94	1.95
	assign (segid 3A4 and resid 107 and name CB)	(segid 3A4 and resid 133 and name CB)	16.84	2.12	2.13
	assign (segid 3A4 and resid 107 and name CB)	(segid 3A4 and resid 260 and name CA)	18.43	0.76	0.76
	assign (segid 3A4 and resid 107 and name CB)	(segid 3A4 and resid 263 and name CA)	17.69	0.48	0.48
	assign (segid 3A4 and resid 107 and name CB)	(segid 3A4 and resid 263 and name CB)	16.42	0.53	0.53
10	assign (segid 3A4 and resid 107 and name CB)	(segid 3A4 and resid 264 and name CA)	18.69	0.41	0.41
	assign (segid 3A4 and resid 107 and name CB)	(segid 3A4 and resid 267 and name CA)	18.53	0.41	0.41
	assign (segid 3A4 and resid 107 and name CB)	(segid 3A4 and resid 267 and name CB)	17.33	0.41	0.40
	assign (segid 3A4 and resid 107 and name CB)	(segid 3A4 and resid 400 and name CA)	16.44	0.71	0.72
	assign (segid 3A4 and resid 107 and name CB)	(segid 3A4 and resid 400 and name CB)	16.68	0.77	0.77
15	assign (segid 3A4 and resid 107 and name CB)	(segid 3A4 and resid 401 and name CA)	17.40	0.44	0.44
	assign (segid 3A4 and resid 107 and name CB)	(segid 3A4 and resid 402 and name CA)	17.69	0.45	0.45
	assign (segid 3A4 and resid 107 and name CB)	(segid 3A4 and resid 402 and name CB)	18.75	0.54	0.53
	assign (segid 3A4 and resid 107 and name CB)	(segid 3A4 and resid 403 and name CA)	14.46	0.53	0.52
	assign (segid 3A4 and resid 107 and name CB)	(segid 3A4 and resid 403 and name CB)	14.18	0.67	0.67
20	assign (segid 3A4 and resid 107 and name CB)	(segid 3A4 and resid 404 and name CA)	12.59	0.38	0.38
	assign (segid 3A4 and resid 107 and name CB)	(segid 3A4 and resid 404 and name CB)	12.99	0.46	0.47
	assign (segid 3A4 and resid 107 and name CB)	(segid 3A4 and resid 405 and name CA)	14.81	0.56	0.56
	assign (segid 3A4 and resid 107 and name CB)	(segid 3A4 and resid 405 and name CB)	16.28	0.55	0.54
	assign (segid 3A4 and resid 107 and name CB)	(segid 3A4 and resid 406 and name CA)	14.81	0.66	0.66
25	assign (segid 3A4 and resid 107 and name CB)	(segid 3A4 and resid 407 and name CA)	11.15	0.71	0.71
	assign (segid 3A4 and resid 107 and name CB)	(segid 3A4 and resid 407 and name CB)	10.19	0.59	0.59
	assign (segid 3A4 and resid 107 and name CB)	(segid 3A4 and resid 408 and name CA)	11.02	0.82	0.83
	assign (segid 3A4 and resid 107 and name CB)	(segid 3A4 and resid 408 and name CB)	11.65	0.85	0.85
	assign (segid 3A4 and resid 107 and name CB)	(segid 3A4 and resid 409 and name CA)	14.08	0.99	0.99
30	assign (segid 3A4 and resid 107 and name CB)	(segid 3A4 and resid 409 and name CB)	15.43	0.92	0.92
	assign (segid 3A4 and resid 107 and name CB)	(segid 3A4 and resid 410 and name CA)	13.33	1.24	1.23
	assign (segid 3A4 and resid 107 and name CB)	(segid 3A4 and resid 411 and name CA)	10.53	1.40	1.39
	assign (segid 3A4 and resid 107 and name CB)	(segid 3A4 and resid 411 and name CB)	9.11	1.36	1.36
	assign (segid 3A4 and resid 107 and name CB)	(segid 3A4 and resid 412 and name CA)	12.53	1.44	1.44
35	assign (segid 3A4 and resid 107 and name CB)	(segid 3A4 and resid 414 and name CA)	17.30	1.17	1.16
	assign (segid 3A4 and resid 107 and name CB)	(segid 3A4 and resid 440 and name CA)	17.43	0.76	0.75
	assign (segid 3A4 and resid 107 and name N)	(segid 3A4 and resid 107 and name C)	2.47	0.04	0.03
	assign (segid 3A4 and resid 107 and name N)	(segid 3A4 and resid 107 and name CA)	1.46	0.02	0.02
40	assign (segid 3A4 and resid 107 and name N)	(segid 3A4 and resid 107 and name CB)	2.46	0.03	0.02
	assign (segid 3A4 and resid 107 and name N)	(segid 3A4 and resid 108 and name C)	3.48	0.05	0.05
	assign (segid 3A4 and resid 107 and name N)	(segid 3A4 and resid 108 and name CA)	4.21	0.06	0.04
	assign (segid 3A4 and resid 107 and name N)	(segid 3A4 and resid 108 and name CB)	4.93	0.11	0.12
	assign (segid 3A4 and resid 107 and name N)	(segid 3A4 and resid 108 and name N)	2.84	0.06	0.06
45	assign (segid 3A4 and resid 107 and name N)	(segid 3A4 and resid 108 and name O)	5.81	0.08	0.08
	assign (segid 3A4 and resid 107 and name N)	(segid 3A4 and resid 109 and name C)	5.54	0.05	0.05
	assign (segid 3A4 and resid 107 and name N)	(segid 3A4 and resid 109 and name CA)	5.28	0.07	0.08
	assign (segid 3A4 and resid 107 and name N)	(segid 3A4 and resid 109 and name CB)	5.38	0.13	0.14
	assign (segid 3A4 and resid 107 and name N)	(segid 3A4 and resid 109 and name N)	4.27	0.06	0.06
50	assign (segid 3A4 and resid 107 and name N)	(segid 3A4 and resid 109 and name O)	6.74	0.05	0.05
	assign (segid 3A4 and resid 107 and name N)	(segid 3A4 and resid 110 and name C)	6.50	0.18	0.17
	assign (segid 3A4 and resid 107 and name N)	(segid 3A4 and resid 110 and name CA)	5.49	0.07	0.06
	assign (segid 3A4 and resid 107 and name N)	(segid 3A4 and resid 110 and name CB)	4.90	0.07	0.07
	assign (segid 3A4 and resid 107 and name N)	(segid 3A4 and resid 110 and name N)	4.73	0.07	0.07
55	assign (segid 3A4 and resid 107 and name N)	(segid 3A4 and resid 110 and name O)	7.61	0.16	0.16
	assign (segid 3A4 and resid 107 and name N)	(segid 3A4 and resid 111 and name N)	6.35	0.28	0.28
	assign (segid 3A4 and resid 107 and name N)	(segid 3A4 and resid 107 and name CB)	3.28	0.08	0.09
	assign (segid 3A4 and resid 107 and name O)	(segid 3A4 and resid 108 and name C)	2.94	0.07	0.06
	assign (segid 3A4 and resid 107 and name O)	(segid 3A4 and resid 108 and name CA)	2.77	0.04	0.04
60	assign (segid 3A4 and resid 107 and name O)	(segid 3A4 and resid 108 and name CB)	4.24	0.04	0.04
	assign (segid 3A4 and resid 107 and name O)	(segid 3A4 and resid 108 and name N)	2.23	0.02	0.03
	assign (segid 3A4 and resid 107 and name O)	(segid 3A4 and resid 108 and name O)	3.47	0.16	0.16
	assign (segid 3A4 and resid 107 and name O)	(segid 3A4 and resid 109 and name C)	3.97	0.15	0.15
	assign (segid 3A4 and resid 107 and name O)	(segid 3A4 and resid 109 and name CA)	4.27	0.10	0.11
65	assign (segid 3A4 and resid 107 and name O)	(segid 3A4 and resid 109 and name CB)	5.29	0.17	0.16
	assign (segid 3A4 and resid 107 and name O)	(segid 3A4 and resid 109 and name N)	3.32	0.11	0.12
	assign (segid 3A4 and resid 107 and name O)	(segid 3A4 and resid 109 and name O)	4.90	0.16	0.16
	assign (segid 3A4 and resid 107 and name O)	(segid 3A4 and resid 110 and name C)	3.88	0.37	0.36
	assign (segid 3A4 and resid 107 and name O)	(segid 3A4 and resid 110 and name CA)	3.60	0.27	0.26
70	assign (segid 3A4 and resid 107 and name O)	(segid 3A4 and resid 110 and name CB)	3.38	0.29	0.28
	assign (segid 3A4 and resid 107 and name O)	(segid 3A4 and resid 110 and name N)	3.13	0.25	0.25
	assign (segid 3A4 and resid 107 and name O)	(segid 3A4 and resid 110 and name O)	5.03	0.39	0.40
	assign (segid 3A4 and resid 107 and name O)	(segid 3A4 and resid 111 and name C)	5.42	0.42	0.43
	assign (segid 3A4 and resid 107 and name O)	(segid 3A4 and resid 111 and name CA)	4.26	0.49	0.49
75	assign (segid 3A4 and resid 107 and name O)	(segid 3A4 and resid 111 and name CB)	4.02	0.50	0.50
	assign (segid 3A4 and resid 107 and name O)	(segid 3A4 and resid 111 and name N)	3.27	0.43	0.43
	assign (segid 3A4 and resid 107 and name O)	(segid 3A4 and resid 111 and name O)	6.40	0.55	0.54
	assign (segid 3A4 and resid 107 and name O)	(segid 3A4 and resid 112 and name CA)	6.98	0.26	0.26
	assign (segid 3A4 and resid 107 and name O)	(segid 3A4 and resid 112 and name N)	5.65	0.31	0.31
80	assign (segid 3A4 and resid 107 and name O)	(segid 3A4 and resid 112 and name CB)	2.51	0.04	0.04
	assign (segid 3A4 and resid 108 and name C)	(segid 3A4 and resid 108 and name O)	1.24	0.01	0.01
	assign (segid 3A4 and resid 108 and name C)	(segid 3A4 and resid 109 and name C)	3.07	0.09	0.09

	assign (segid 3A4 and resid 108 and name C)	(segid 3A4 and resid 109 and name CA)	2.43	0.02	0.02
	assign (segid 3A4 and resid 108 and name C)	(segid 3A4 and resid 109 and name CB)	3.69	0.03	0.02
	assign (segid 3A4 and resid 108 and name C)	(segid 3A4 and resid 109 and name N)	1.33	0.00	0.00
	assign (segid 3A4 and resid 108 and name C)	(segid 3A4 and resid 109 and name O)	3.94	0.12	0.11
5	assign (segid 3A4 and resid 108 and name C)	(segid 3A4 and resid 110 and name C)	4.72	0.30	0.30
	assign (segid 3A4 and resid 108 and name C)	(segid 3A4 and resid 110 and name CA)	4.50	0.16	0.17
	assign (segid 3A4 and resid 108 and name C)	(segid 3A4 and resid 110 and name CB)	5.17	0.14	0.14
	assign (segid 3A4 and resid 108 and name C)	(segid 3A4 and resid 110 and name N)	3.30	0.15	0.15
	assign (segid 3A4 and resid 108 and name C)	(segid 3A4 and resid 110 and name O)	5.86	0.30	0.30
10	assign (segid 3A4 and resid 108 and name C)	(segid 3A4 and resid 111 and name C)	5.23	0.50	0.50
	assign (segid 3A4 and resid 108 and name C)	(segid 3A4 and resid 111 and name CA)	4.80	0.50	0.51
	assign (segid 3A4 and resid 108 and name C)	(segid 3A4 and resid 111 and name CB)	4.64	0.55	0.55
	assign (segid 3A4 and resid 108 and name C)	(segid 3A4 and resid 111 and name N)	3.98	0.42	0.42
	assign (segid 3A4 and resid 108 and name C)	(segid 3A4 and resid 111 and name O)	6.14	0.68	0.68
15	assign (segid 3A4 and resid 108 and name C)	(segid 3A4 and resid 112 and name C)	7.14	0.28	0.29
	assign (segid 3A4 and resid 108 and name C)	(segid 3A4 and resid 112 and name CA)	5.94	0.31	0.31
	assign (segid 3A4 and resid 108 and name C)	(segid 3A4 and resid 112 and name N)	5.01	0.37	0.37
	assign (segid 3A4 and resid 108 and name CA)	(segid 3A4 and resid 108 and name C)	1.52	0.01	0.01
	assign (segid 3A4 and resid 108 and name CA)	(segid 3A4 and resid 108 and name CB)	1.52	0.01	0.01
20	assign (segid 3A4 and resid 108 and name CA)	(segid 3A4 and resid 108 and name O)	2.39	0.00	0.01
	assign (segid 3A4 and resid 108 and name CA)	(segid 3A4 and resid 109 and name C)	4.43	0.08	0.08
	assign (segid 3A4 and resid 108 and name CA)	(segid 3A4 and resid 109 and name CA)	3.81	0.01	0.01
	assign (segid 3A4 and resid 108 and name CA)	(segid 3A4 and resid 109 and name CB)	4.84	0.03	0.03
	assign (segid 3A4 and resid 108 and name CA)	(segid 3A4 and resid 109 and name N)	2.44	0.01	0.01
25	assign (segid 3A4 and resid 108 and name CA)	(segid 3A4 and resid 109 and name O)	5.38	0.11	0.10
	assign (segid 3A4 and resid 108 and name CA)	(segid 3A4 and resid 110 and name C)	5.64	0.34	0.35
	assign (segid 3A4 and resid 108 and name CA)	(segid 3A4 and resid 110 and name CA)	5.43	0.18	0.19
	assign (segid 3A4 and resid 108 and name CA)	(segid 3A4 and resid 110 and name CB)	5.74	0.19	0.19
	assign (segid 3A4 and resid 108 and name CA)	(segid 3A4 and resid 110 and name N)	4.35	0.15	0.16
30	assign (segid 3A4 and resid 108 and name CA)	(segid 3A4 and resid 110 and name O)	6.81	0.35	0.35
	assign (segid 3A4 and resid 108 and name CA)	(segid 3A4 and resid 111 and name C)	6.13	0.58	0.58
	assign (segid 3A4 and resid 108 and name CA)	(segid 3A4 and resid 111 and name CA)	5.48	0.61	0.61
	assign (segid 3A4 and resid 108 and name CA)	(segid 3A4 and resid 111 and name CB)	4.93	0.70	0.70
	assign (segid 3A4 and resid 108 and name CA)	(segid 3A4 and resid 111 and name N)	4.78	0.48	0.48
35	assign (segid 3A4 and resid 108 and name CA)	(segid 3A4 and resid 112 and name CA)	7.17	0.36	0.36
	assign (segid 3A4 and resid 108 and name CA)	(segid 3A4 and resid 112 and name N)	6.16	0.41	0.41
	assign (segid 3A4 and resid 108 and name CA)	(segid 3A4 and resid 119 and name CA)	11.06	0.75	0.75
	assign (segid 3A4 and resid 108 and name CA)	(segid 3A4 and resid 119 and name CB)	9.81	0.56	0.57
40	assign (segid 3A4 and resid 108 and name CA)	(segid 3A4 and resid 120 and name CA)	12.49	0.46	0.45
	assign (segid 3A4 and resid 108 and name CA)	(segid 3A4 and resid 120 and name CB)	13.09	0.59	0.60
	assign (segid 3A4 and resid 108 and name CA)	(segid 3A4 and resid 121 and name CA)	11.40	0.75	0.74
	assign (segid 3A4 and resid 108 and name CA)	(segid 3A4 and resid 121 and name CB)	12.13	0.81	0.81
	assign (segid 3A4 and resid 108 and name CA)	(segid 3A4 and resid 122 and name CA)	13.33	1.10	1.09
	assign (segid 3A4 and resid 108 and name CA)	(segid 3A4 and resid 122 and name CB)	14.76	1.09	1.08
45	assign (segid 3A4 and resid 108 and name CA)	(segid 3A4 and resid 123 and name CA)	11.91	0.87	0.88
	assign (segid 3A4 and resid 108 and name CA)	(segid 3A4 and resid 123 and name CB)	12.30	0.89	0.89
	assign (segid 3A4 and resid 108 and name CA)	(segid 3A4 and resid 124 and name CA)	8.39	0.81	0.82
	assign (segid 3A4 and resid 108 and name CA)	(segid 3A4 and resid 124 and name CB)	7.77	0.67	0.67
	assign (segid 3A4 and resid 108 and name CA)	(segid 3A4 and resid 125 and name CA)	9.15	1.65	1.64
50	assign (segid 3A4 and resid 108 and name CA)	(segid 3A4 and resid 125 and name CB)	9.38	1.94	1.95
	assign (segid 3A4 and resid 108 and name CA)	(segid 3A4 and resid 126 and name CA)	12.26	1.40	1.41
	assign (segid 3A4 and resid 108 and name CA)	(segid 3A4 and resid 127 and name CA)	12.12	1.33	1.32
	assign (segid 3A4 and resid 108 and name CA)	(segid 3A4 and resid 127 and name CB)	11.89	1.72	1.71
	assign (segid 3A4 and resid 108 and name CA)	(segid 3A4 and resid 128 and name CA)	10.60	1.15	1.14
55	assign (segid 3A4 and resid 108 and name CA)	(segid 3A4 and resid 128 and name CB)	9.58	1.17	1.16
	assign (segid 3A4 and resid 108 and name CA)	(segid 3A4 and resid 129 and name CA)	11.93	1.97	1.97
	assign (segid 3A4 and resid 108 and name CA)	(segid 3A4 and resid 129 and name CB)	12.03	2.27	2.26
	assign (segid 3A4 and resid 108 and name CA)	(segid 3A4 and resid 130 and name CA)	14.82	1.34	1.35
	assign (segid 3A4 and resid 108 and name CA)	(segid 3A4 and resid 130 and name CB)	15.29	1.29	1.29
60	assign (segid 3A4 and resid 108 and name CA)	(segid 3A4 and resid 131 and name CA)	14.70	1.34	1.33
	assign (segid 3A4 and resid 108 and name CA)	(segid 3A4 and resid 131 and name CB)	14.07	1.57	1.56
	assign (segid 3A4 and resid 108 and name CA)	(segid 3A4 and resid 132 and name CA)	14.16	1.48	1.48
	assign (segid 3A4 and resid 108 and name CA)	(segid 3A4 and resid 132 and name CB)	13.21	1.82	1.82
	assign (segid 3A4 and resid 108 and name CA)	(segid 3A4 and resid 133 and name CA)	16.55	1.84	1.84
65	assign (segid 3A4 and resid 108 and name CA)	(segid 3A4 and resid 133 and name CB)	16.69	2.01	2.01
	assign (segid 3A4 and resid 108 and name CA)	(segid 3A4 and resid 135 and name CB)	17.35	1.21	1.20
	assign (segid 3A4 and resid 108 and name CA)	(segid 3A4 and resid 260 and name CA)	16.40	1.19	1.19
	assign (segid 3A4 and resid 108 and name CA)	(segid 3A4 and resid 260 and name CB)	16.32	1.27	1.28
	assign (segid 3A4 and resid 108 and name CA)	(segid 3A4 and resid 263 and name CA)	16.13	1.13	1.13
70	assign (segid 3A4 and resid 108 and name CA)	(segid 3A4 and resid 263 and name CB)	14.87	1.17	1.17
	assign (segid 3A4 and resid 108 and name CA)	(segid 3A4 and resid 264 and name CA)	16.40	1.01	1.02
	assign (segid 3A4 and resid 108 and name CA)	(segid 3A4 and resid 267 and name CA)	16.82	0.72	0.72
	assign (segid 3A4 and resid 108 and name CA)	(segid 3A4 and resid 267 and name CB)	15.44	0.71	0.72
	assign (segid 3A4 and resid 108 and name CA)	(segid 3A4 and resid 400 and name CA)	16.82	1.24	1.25
75	assign (segid 3A4 and resid 108 and name CA)	(segid 3A4 and resid 400 and name CB)	16.79	1.26	1.25
	assign (segid 3A4 and resid 108 and name CA)	(segid 3A4 and resid 401 and name CA)	17.37	1.10	1.10
	assign (segid 3A4 and resid 108 and name CA)	(segid 3A4 and resid 402 and name CA)	18.40	1.10	1.10
	assign (segid 3A4 and resid 108 and name CA)	(segid 3A4 and resid 403 and name CA)	15.66	1.12	1.12
	assign (segid 3A4 and resid 108 and name CA)	(segid 3A4 and resid 403 and name CB)	15.50	1.20	1.19
80	assign (segid 3A4 and resid 108 and name CA)	(segid 3A4 and resid 404 and name CA)	12.97	1.11	1.11
	assign (segid 3A4 and resid 108 and name CA)	(segid 3A4 and resid 404 and name CB)	12.95	1.18	1.18
	assign (segid 3A4 and resid 108 and name CA)	(segid 3A4 and resid 405 and name CA)	15.02	1.14	1.14
	assign (segid 3A4 and resid 108 and name CA)	(segid 3A4 and resid 405 and name CB)	16.38	1.13	1.12

	assign (segid 3A4 and resid 108 and name CA)	(segid 3A4 and resid 406 and name CA)	15.97	0.97	0.96
	assign (segid 3A4 and resid 108 and name CA)	(segid 3A4 and resid 407 and name CA)	12.60	0.91	0.91
	assign (segid 3A4 and resid 108 and name CA)	(segid 3A4 and resid 407 and name CB)	11.76	1.00	1.00
	assign (segid 3A4 and resid 108 and name CA)	(segid 3A4 and resid 408 and name CA)	11.31	0.69	0.70
	assign (segid 3A4 and resid 108 and name CA)	(segid 3A4 and resid 408 and name CB)	11.45	0.82	0.82
5	assign (segid 3A4 and resid 108 and name CA)	(segid 3A4 and resid 409 and name CA)	14.53	0.42	0.42
	assign (segid 3A4 and resid 108 and name CA)	(segid 3A4 and resid 409 and name CB)	15.84	0.47	0.48
	assign (segid 3A4 and resid 108 and name CA)	(segid 3A4 and resid 410 and name CA)	14.77	0.43	0.43
	assign (segid 3A4 and resid 108 and name CA)	(segid 3A4 and resid 411 and name CA)	11.76	0.36	0.36
	assign (segid 3A4 and resid 108 and name CA)	(segid 3A4 and resid 411 and name CB)	10.38	0.38	0.38
10	assign (segid 3A4 and resid 108 and name CA)	(segid 3A4 and resid 412 and name CA)	12.55	0.56	0.56
	assign (segid 3A4 and resid 108 and name CA)	(segid 3A4 and resid 413 and name CA)	16.30	0.89	0.89
	assign (segid 3A4 and resid 108 and name CA)	(segid 3A4 and resid 414 and name CA)	15.77	0.87	0.87
	assign (segid 3A4 and resid 108 and name CA)	(segid 3A4 and resid 415 and name CA)	17.79	0.51	0.52
	assign (segid 3A4 and resid 108 and name CA)	(segid 3A4 and resid 416 and name CA)	18.70	0.16	0.16
15	assign (segid 3A4 and resid 108 and name CA)	(segid 3A4 and resid 438 and name CA)	17.05	0.77	0.77
	assign (segid 3A4 and resid 108 and name CA)	(segid 3A4 and resid 439 and name CA)	15.74	0.37	0.38
	assign (segid 3A4 and resid 108 and name CA)	(segid 3A4 and resid 440 and name CA)	14.49	0.22	0.22
	assign (segid 3A4 and resid 108 and name CA)	(segid 3A4 and resid 109 and name C)	5.48	0.13	0.12
	assign (segid 3A4 and resid 108 and name CB)	(segid 3A4 and resid 109 and name CA)	4.51	0.12	0.12
20	assign (segid 3A4 and resid 108 and name CB)	(segid 3A4 and resid 109 and name CB)	5.32	0.16	0.16
	assign (segid 3A4 and resid 108 and name CB)	(segid 3A4 and resid 109 and name N)	3.20	0.12	0.12
	assign (segid 3A4 and resid 108 and name CB)	(segid 3A4 and resid 109 and name O)	6.39	0.14	0.15
	assign (segid 3A4 and resid 108 and name CB)	(segid 3A4 and resid 110 and name C)	7.05	0.35	0.35
	assign (segid 3A4 and resid 108 and name CB)	(segid 3A4 and resid 110 and name CA)	6.80	0.17	0.17
25	assign (segid 3A4 and resid 108 and name CB)	(segid 3A4 and resid 110 and name CB)	7.16	0.15	0.15
	assign (segid 3A4 and resid 108 and name CB)	(segid 3A4 and resid 110 and name N)	5.60	0.14	0.15
	assign (segid 3A4 and resid 108 and name CB)	(segid 3A4 and resid 111 and name CA)	6.79	0.66	0.66
	assign (segid 3A4 and resid 108 and name CB)	(segid 3A4 and resid 111 and name CB)	6.17	0.78	0.79
	assign (segid 3A4 and resid 108 and name CB)	(segid 3A4 and resid 111 and name N)	6.19	0.50	0.50
30	assign (segid 3A4 and resid 108 and name CB)	(segid 3A4 and resid 112 and name CA)	8.07	0.47	0.46
	assign (segid 3A4 and resid 108 and name CB)	(segid 3A4 and resid 119 and name CA)	11.11	0.88	0.88
	assign (segid 3A4 and resid 108 and name CB)	(segid 3A4 and resid 119 and name CB)	9.90	0.65	0.65
	assign (segid 3A4 and resid 108 and name CB)	(segid 3A4 and resid 120 and name CA)	12.13	0.66	0.65
	assign (segid 3A4 and resid 108 and name CB)	(segid 3A4 and resid 120 and name CB)	12.63	0.79	0.80
35	assign (segid 3A4 and resid 108 and name CB)	(segid 3A4 and resid 121 and name CA)	10.94	0.83	0.84
	assign (segid 3A4 and resid 108 and name CB)	(segid 3A4 and resid 121 and name CB)	11.75	0.91	0.91
	assign (segid 3A4 and resid 108 and name CB)	(segid 3A4 and resid 122 and name CA)	12.51	1.20	1.21
	assign (segid 3A4 and resid 108 and name CB)	(segid 3A4 and resid 122 and name CB)	13.94	1.20	1.19
	assign (segid 3A4 and resid 108 and name CB)	(segid 3A4 and resid 123 and name CA)	10.97	0.91	0.92
40	assign (segid 3A4 and resid 108 and name CB)	(segid 3A4 and resid 123 and name CB)	11.42	0.96	0.95
	assign (segid 3A4 and resid 108 and name CB)	(segid 3A4 and resid 124 and name CA)	7.56	0.81	0.80
	assign (segid 3A4 and resid 108 and name CB)	(segid 3A4 and resid 124 and name CB)	7.14	0.76	0.76
	assign (segid 3A4 and resid 108 and name CB)	(segid 3A4 and resid 125 and name CA)	8.22	1.69	1.70
	assign (segid 3A4 and resid 108 and name CB)	(segid 3A4 and resid 125 and name CB)	8.64	1.93	1.93
45	assign (segid 3A4 and resid 108 and name CB)	(segid 3A4 and resid 126 and name CA)	11.21	1.54	1.53
	assign (segid 3A4 and resid 108 and name CB)	(segid 3A4 and resid 127 and name CA)	10.87	1.49	1.49
	assign (segid 3A4 and resid 108 and name CB)	(segid 3A4 and resid 127 and name CB)	10.65	1.87	1.87
	assign (segid 3A4 and resid 108 and name CB)	(segid 3A4 and resid 128 and name CA)	9.35	1.17	1.18
	assign (segid 3A4 and resid 108 and name CB)	(segid 3A4 and resid 128 and name CB)	8.38	1.18	1.19
50	assign (segid 3A4 and resid 108 and name CB)	(segid 3A4 and resid 129 and name CA)	10.75	2.05	2.05
	assign (segid 3A4 and resid 108 and name CB)	(segid 3A4 and resid 129 and name CB)	10.91	2.33	2.34
	assign (segid 3A4 and resid 108 and name CB)	(segid 3A4 and resid 130 and name CA)	13.58	1.44	1.45
	assign (segid 3A4 and resid 108 and name CB)	(segid 3A4 and resid 130 and name CB)	14.05	1.45	1.44
	assign (segid 3A4 and resid 108 and name CB)	(segid 3A4 and resid 131 and name CA)	13.42	1.35	1.35
55	assign (segid 3A4 and resid 108 and name CB)	(segid 3A4 and resid 131 and name CB)	12.79	1.56	1.55
	assign (segid 3A4 and resid 108 and name CB)	(segid 3A4 and resid 132 and name CA)	12.97	1.44	1.45
	assign (segid 3A4 and resid 108 and name CB)	(segid 3A4 and resid 132 and name CB)	12.06	1.80	1.80
	assign (segid 3A4 and resid 108 and name CB)	(segid 3A4 and resid 133 and name CA)	15.38	1.82	1.83
	assign (segid 3A4 and resid 108 and name CB)	(segid 3A4 and resid 133 and name CB)	15.53	1.99	1.99
60	assign (segid 3A4 and resid 108 and name CB)	(segid 3A4 and resid 134 and name CA)	17.33	1.30	1.30
	assign (segid 3A4 and resid 108 and name CB)	(segid 3A4 and resid 135 and name CA)	17.16	1.08	1.08
	assign (segid 3A4 and resid 108 and name CB)	(segid 3A4 and resid 135 and name CB)	16.19	1.07	1.07
	assign (segid 3A4 and resid 108 and name CB)	(segid 3A4 and resid 136 and name CA)	18.08	1.42	1.42
	assign (segid 3A4 and resid 108 and name CB)	(segid 3A4 and resid 259 and name CB)	17.16	1.50	1.50
65	assign (segid 3A4 and resid 108 and name CB)	(segid 3A4 and resid 260 and name CA)	15.35	1.39	1.39
	assign (segid 3A4 and resid 108 and name CB)	(segid 3A4 and resid 260 and name CB)	15.21	1.45	1.46
	assign (segid 3A4 and resid 108 and name CB)	(segid 3A4 and resid 263 and name CA)	15.43	1.40	1.40
	assign (segid 3A4 and resid 108 and name CB)	(segid 3A4 and resid 263 and name CB)	14.12	1.43	1.43
	assign (segid 3A4 and resid 108 and name CB)	(segid 3A4 and resid 264 and name CA)	15.76	1.28	1.28
70	assign (segid 3A4 and resid 108 and name CB)	(segid 3A4 and resid 267 and name CA)	16.58	0.98	0.99
	assign (segid 3A4 and resid 108 and name CB)	(segid 3A4 and resid 267 and name CB)	15.19	0.97	0.97
	assign (segid 3A4 and resid 108 and name CB)	(segid 3A4 and resid 400 and name CA)	16.08	1.44	1.44
	assign (segid 3A4 and resid 108 and name CB)	(segid 3A4 and resid 400 and name CB)	15.94	1.44	1.45
	assign (segid 3A4 and resid 108 and name CB)	(segid 3A4 and resid 401 and name CA)	16.74	1.36	1.37
75	assign (segid 3A4 and resid 108 and name CB)	(segid 3A4 and resid 402 and name CA)	18.02	1.34	1.34
	assign (segid 3A4 and resid 108 and name CB)	(segid 3A4 and resid 403 and name CA)	15.33	1.31	1.31
	assign (segid 3A4 and resid 108 and name CB)	(segid 3A4 and resid 403 and name CB)	15.10	1.36	1.36
	assign (segid 3A4 and resid 108 and name CB)	(segid 3A4 and resid 404 and name CA)	12.60	1.36	1.36
	assign (segid 3A4 and resid 108 and name CB)	(segid 3A4 and resid 404 and name CB)	12.45	1.45	1.46
80	assign (segid 3A4 and resid 108 and name CB)	(segid 3A4 and resid 405 and name CA)	14.85	1.39	1.40
	assign (segid 3A4 and resid 108 and name CB)	(segid 3A4 and resid 405 and name CB)	16.16	1.40	1.41
	assign (segid 3A4 and resid 108 and name CB)	(segid 3A4 and resid 406 and name CA)	16.02	1.18	1.19

	assign (segid 3A4 and resid 108 and name CB)	(segid 3A4 and resid 407 and name CA)	12.80	1.09	1.09
	assign (segid 3A4 and resid 108 and name CB)	(segid 3A4 and resid 407 and name CB)	11.87	1.17	1.18
	assign (segid 3A4 and resid 108 and name CB)	(segid 3A4 and resid 408 and name CA)	11.56	0.89	0.89
	assign (segid 3A4 and resid 108 and name CB)	(segid 3A4 and resid 408 and name CB)	11.56	1.00	1.01
5	assign (segid 3A4 and resid 108 and name CB)	(segid 3A4 and resid 409 and name CA)	14.94	0.66	0.67
	assign (segid 3A4 and resid 108 and name CB)	(segid 3A4 and resid 409 and name CB)	16.18	0.74	0.75
	assign (segid 3A4 and resid 108 and name CB)	(segid 3A4 and resid 410 and name CA)	15.38	0.56	0.56
	assign (segid 3A4 and resid 108 and name CB)	(segid 3A4 and resid 411 and name CA)	12.59	0.37	0.37
	assign (segid 3A4 and resid 108 and name CB)	(segid 3A4 and resid 411 and name CB)	11.19	0.41	0.40
10	assign (segid 3A4 and resid 108 and name CB)	(segid 3A4 and resid 412 and name CA)	13.35	0.48	0.49
	assign (segid 3A4 and resid 108 and name CB)	(segid 3A4 and resid 413 and name CA)	17.03	0.81	0.82
	assign (segid 3A4 and resid 108 and name CB)	(segid 3A4 and resid 414 and name CA)	16.27	1.02	1.02
	assign (segid 3A4 and resid 108 and name CB)	(segid 3A4 and resid 415 and name CA)	18.17	0.61	0.61
	assign (segid 3A4 and resid 108 and name CB)	(segid 3A4 and resid 416 and name CA)	18.89	0.39	0.39
15	assign (segid 3A4 and resid 108 and name CB)	(segid 3A4 and resid 438 and name CA)	16.66	0.93	0.94
	assign (segid 3A4 and resid 108 and name CB)	(segid 3A4 and resid 439 and name CA)	15.62	0.63	0.64
	assign (segid 3A4 and resid 108 and name CB)	(segid 3A4 and resid 440 and name CA)	14.64	0.39	0.40
	assign (segid 3A4 and resid 108 and name CB)	(segid 3A4 and resid 108 and name C)	2.44	0.01	0.02
	assign (segid 3A4 and resid 108 and name N)	(segid 3A4 and resid 108 and name CA)	1.45	0.01	0.00
20	assign (segid 3A4 and resid 108 and name N)	(segid 3A4 and resid 108 and name CB)	2.43	0.02	0.02
	assign (segid 3A4 and resid 108 and name N)	(segid 3A4 and resid 108 and name O)	3.50	0.06	0.05
	assign (segid 3A4 and resid 108 and name N)	(segid 3A4 and resid 109 and name C)	4.68	0.05	0.05
	assign (segid 3A4 and resid 108 and name N)	(segid 3A4 and resid 109 and name CA)	4.20	0.04	0.04
	assign (segid 3A4 and resid 108 and name N)	(segid 3A4 and resid 109 and name CB)	4.97	0.04	0.04
25	assign (segid 3A4 and resid 108 and name N)	(segid 3A4 and resid 109 and name N)	2.80	0.06	0.05
	assign (segid 3A4 and resid 108 and name N)	(segid 3A4 and resid 109 and name O)	5.78	0.07	0.07
	assign (segid 3A4 and resid 108 and name N)	(segid 3A4 and resid 110 and name C)	5.72	0.27	0.27
	assign (segid 3A4 and resid 108 and name N)	(segid 3A4 and resid 110 and name CA)	5.24	0.12	0.12
	assign (segid 3A4 and resid 108 and name N)	(segid 3A4 and resid 110 and name CB)	5.20	0.14	0.14
30	assign (segid 3A4 and resid 108 and name N)	(segid 3A4 and resid 110 and name N)	4.25	0.12	0.12
	assign (segid 3A4 and resid 108 and name N)	(segid 3A4 and resid 110 and name O)	6.92	0.27	0.27
	assign (segid 3A4 and resid 108 and name N)	(segid 3A4 and resid 111 and name CA)	5.96	0.52	0.51
	assign (segid 3A4 and resid 108 and name N)	(segid 3A4 and resid 111 and name CB)	5.49	0.60	0.60
	assign (segid 3A4 and resid 108 and name N)	(segid 3A4 and resid 111 and name N)	5.05	0.41	0.41
35	assign (segid 3A4 and resid 108 and name N)	(segid 3A4 and resid 112 and name N)	6.92	0.32	0.32
	assign (segid 3A4 and resid 108 and name O)	(segid 3A4 and resid 108 and name CB)	3.27	0.07	0.08
	assign (segid 3A4 and resid 108 and name O)	(segid 3A4 and resid 109 and name C)	3.09	0.15	0.15
	assign (segid 3A4 and resid 108 and name O)	(segid 3A4 and resid 109 and name CA)	2.75	0.03	0.03
	assign (segid 3A4 and resid 108 and name O)	(segid 3A4 and resid 109 and name CB)	4.21	0.03	0.03
40	assign (segid 3A4 and resid 108 and name O)	(segid 3A4 and resid 109 and name N)	2.25	0.01	0.00
	assign (segid 3A4 and resid 108 and name O)	(segid 3A4 and resid 109 and name O)	3.61	0.19	0.19
	assign (segid 3A4 and resid 108 and name O)	(segid 3A4 and resid 110 and name C)	4.41	0.41	0.40
	assign (segid 3A4 and resid 108 and name O)	(segid 3A4 and resid 110 and name CA)	4.55	0.25	0.26
	assign (segid 3A4 and resid 108 and name O)	(segid 3A4 and resid 110 and name CB)	5.43	0.20	0.20
45	assign (segid 3A4 and resid 108 and name O)	(segid 3A4 and resid 110 and name N)	3.55	0.20	0.20
	assign (segid 3A4 and resid 108 and name O)	(segid 3A4 and resid 110 and name O)	5.42	0.42	0.42
	assign (segid 3A4 and resid 108 and name O)	(segid 3A4 and resid 111 and name C)	4.25	0.61	0.62
	assign (segid 3A4 and resid 108 and name O)	(segid 3A4 and resid 111 and name CA)	4.07	0.60	0.61
	assign (segid 3A4 and resid 108 and name O)	(segid 3A4 and resid 111 and name CB)	3.96	0.60	0.61
50	assign (segid 3A4 and resid 108 and name O)	(segid 3A4 and resid 111 and name N)	3.53	0.51	0.51
	assign (segid 3A4 and resid 108 and name O)	(segid 3A4 and resid 111 and name O)	5.09	0.79	0.79
	assign (segid 3A4 and resid 108 and name O)	(segid 3A4 and resid 112 and name C)	6.16	0.39	0.40
	assign (segid 3A4 and resid 108 and name O)	(segid 3A4 and resid 112 and name CA)	4.88	0.39	0.40
	assign (segid 3A4 and resid 108 and name O)	(segid 3A4 and resid 112 and name N)	4.02	0.47	0.47
55	assign (segid 3A4 and resid 109 and name C)	(segid 3A4 and resid 109 and name CB)	2.52	0.00	0.01
	assign (segid 3A4 and resid 109 and name C)	(segid 3A4 and resid 109 and name O)	1.23	0.01	0.00
	assign (segid 3A4 and resid 109 and name C)	(segid 3A4 and resid 110 and name C)	3.05	0.03	0.03
	assign (segid 3A4 and resid 109 and name C)	(segid 3A4 and resid 110 and name CA)	2.45	0.01	0.01
	assign (segid 3A4 and resid 109 and name C)	(segid 3A4 and resid 110 and name CB)	3.72	0.01	0.01
60	assign (segid 3A4 and resid 109 and name C)	(segid 3A4 and resid 110 and name N)	1.32	0.01	0.02
	assign (segid 3A4 and resid 109 and name C)	(segid 3A4 and resid 110 and name O)	3.96	0.10	0.11
	assign (segid 3A4 and resid 109 and name C)	(segid 3A4 and resid 111 and name C)	4.65	0.04	0.05
	assign (segid 3A4 and resid 109 and name C)	(segid 3A4 and resid 111 and name CA)	4.44	0.07	0.06
	assign (segid 3A4 and resid 109 and name C)	(segid 3A4 and resid 111 and name CB)	5.21	0.10	0.10
65	assign (segid 3A4 and resid 109 and name C)	(segid 3A4 and resid 111 and name N)	3.22	0.07	0.07
	assign (segid 3A4 and resid 109 and name C)	(segid 3A4 and resid 111 and name O)	5.78	0.12	0.13
	assign (segid 3A4 and resid 109 and name C)	(segid 3A4 and resid 112 and name C)	5.53	0.13	0.13
	assign (segid 3A4 and resid 109 and name C)	(segid 3A4 and resid 112 and name CA)	4.81	0.16	0.17
	assign (segid 3A4 and resid 109 and name C)	(segid 3A4 and resid 112 and name N)	3.96	0.15	0.16
70	assign (segid 3A4 and resid 109 and name C)	(segid 3A4 and resid 112 and name O)	6.17	0.45	0.45
	assign (segid 3A4 and resid 109 and name CA)	(segid 3A4 and resid 109 and name C)	1.53	0.01	0.01
	assign (segid 3A4 and resid 109 and name CA)	(segid 3A4 and resid 109 and name CB)	1.53	0.01	0.01
	assign (segid 3A4 and resid 109 and name CA)	(segid 3A4 and resid 109 and name O)	2.38	0.02	0.03
	assign (segid 3A4 and resid 109 and name CA)	(segid 3A4 and resid 110 and name C)	4.46	0.05	0.04
75	assign (segid 3A4 and resid 109 and name CA)	(segid 3A4 and resid 110 and name CA)	3.83	0.02	0.02
	assign (segid 3A4 and resid 109 and name CA)	(segid 3A4 and resid 110 and name CB)	4.87	0.02	0.03
	assign (segid 3A4 and resid 109 and name CA)	(segid 3A4 and resid 110 and name N)	2.45	0.03	0.02
	assign (segid 3A4 and resid 109 and name CA)	(segid 3A4 and resid 110 and name O)	5.43	0.10	0.10
	assign (segid 3A4 and resid 109 and name CA)	(segid 3A4 and resid 111 and name C)	5.59	0.14	0.15
80	assign (segid 3A4 and resid 109 and name CA)	(segid 3A4 and resid 111 and name CA)	5.45	0.15	0.14
	assign (segid 3A4 and resid 109 and name CA)	(segid 3A4 and resid 111 and name CB)	5.92	0.18	0.18
	assign (segid 3A4 and resid 109 and name CA)	(segid 3A4 and resid 111 and name N)	4.35	0.12	0.12
	assign (segid 3A4 and resid 109 and name CA)	(segid 3A4 and resid 111 and name O)	6.63	0.29	0.29

	assign (segid 3A4 and resid 109 and name CA)	(segid 3A4 and resid 112 and name C)	6.48	0.11	0.11
	assign (segid 3A4 and resid 109 and name CA)	(segid 3A4 and resid 112 and name CA)	5.57	0.16	0.16
	assign (segid 3A4 and resid 109 and name CA)	(segid 3A4 and resid 112 and name N)	4.89	0.18	0.18
	assign (segid 3A4 and resid 109 and name CA)	(segid 3A4 and resid 112 and name O)	7.12	0.32	0.33
5	assign (segid 3A4 and resid 109 and name CA)	(segid 3A4 and resid 119 and name CA)	8.43	1.17	1.18
	assign (segid 3A4 and resid 109 and name CA)	(segid 3A4 and resid 119 and name CB)	7.13	1.05	1.05
	assign (segid 3A4 and resid 109 and name CA)	(segid 3A4 and resid 120 and name CA)	10.32	0.77	0.77
	assign (segid 3A4 and resid 109 and name CA)	(segid 3A4 and resid 120 and name CB)	11.24	0.78	0.77
	assign (segid 3A4 and resid 109 and name CA)	(segid 3A4 and resid 121 and name CA)	9.17	0.83	0.83
10	assign (segid 3A4 and resid 109 and name CA)	(segid 3A4 and resid 121 and name CB)	9.64	0.83	0.83
	assign (segid 3A4 and resid 109 and name CA)	(segid 3A4 and resid 122 and name CA)	11.89	0.99	1.00
	assign (segid 3A4 and resid 109 and name CA)	(segid 3A4 and resid 122 and name CB)	13.30	0.98	0.98
	assign (segid 3A4 and resid 109 and name CA)	(segid 3A4 and resid 123 and name CA)	11.25	0.82	0.82
	assign (segid 3A4 and resid 109 and name CA)	(segid 3A4 and resid 123 and name CB)	11.64	0.78	0.78
15	assign (segid 3A4 and resid 109 and name CA)	(segid 3A4 and resid 124 and name CA)	7.80	0.92	0.92
	assign (segid 3A4 and resid 109 and name CA)	(segid 3A4 and resid 124 and name CB)	6.75	0.86	0.85
	assign (segid 3A4 and resid 109 and name CA)	(segid 3A4 and resid 125 and name CA)	8.47	1.56	1.56
	assign (segid 3A4 and resid 109 and name CA)	(segid 3A4 and resid 125 and name CB)	8.19	2.03	2.02
	assign (segid 3A4 and resid 109 and name CA)	(segid 3A4 and resid 126 and name CA)	11.77	1.44	1.44
20	assign (segid 3A4 and resid 109 and name CA)	(segid 3A4 and resid 127 and name CA)	12.46	0.73	0.73
	assign (segid 3A4 and resid 109 and name CA)	(segid 3A4 and resid 127 and name CB)	12.27	1.05	1.04
	assign (segid 3A4 and resid 109 and name CA)	(segid 3A4 and resid 128 and name CA)	11.55	0.59	0.59
	assign (segid 3A4 and resid 109 and name CA)	(segid 3A4 and resid 128 and name CB)	10.50	0.60	0.61
	assign (segid 3A4 and resid 109 and name CA)	(segid 3A4 and resid 129 and name CA)	12.73	1.63	1.63
25	assign (segid 3A4 and resid 109 and name CA)	(segid 3A4 and resid 129 and name CB)	12.48	2.04	2.03
	assign (segid 3A4 and resid 109 and name CA)	(segid 3A4 and resid 130 and name CA)	15.74	1.02	1.03
	assign (segid 3A4 and resid 109 and name CA)	(segid 3A4 and resid 130 and name CB)	16.04	0.88	0.89
	assign (segid 3A4 and resid 109 and name CA)	(segid 3A4 and resid 131 and name CA)	16.15	0.65	0.65
	assign (segid 3A4 and resid 109 and name CA)	(segid 3A4 and resid 131 and name CB)	15.54	0.82	0.82
30	assign (segid 3A4 and resid 109 and name CA)	(segid 3A4 and resid 132 and name CA)	15.91	0.97	0.96
	assign (segid 3A4 and resid 109 and name CA)	(segid 3A4 and resid 132 and name CB)	14.93	1.25	1.26
	assign (segid 3A4 and resid 109 and name CA)	(segid 3A4 and resid 259 and name CA)	18.27	0.85	0.85
	assign (segid 3A4 and resid 109 and name CA)	(segid 3A4 and resid 259 and name CB)	18.02	0.88	0.88
	assign (segid 3A4 and resid 109 and name CA)	(segid 3A4 and resid 260 and name CA)	15.76	0.82	0.81
35	assign (segid 3A4 and resid 109 and name CA)	(segid 3A4 and resid 260 and name CB)	15.84	0.91	0.91
	assign (segid 3A4 and resid 109 and name CA)	(segid 3A4 and resid 261 and name CA)	17.90	0.75	0.76
	assign (segid 3A4 and resid 109 and name CA)	(segid 3A4 and resid 262 and name CA)	18.23	0.83	0.83
	assign (segid 3A4 and resid 109 and name CA)	(segid 3A4 and resid 263 and name CA)	14.59	0.84	0.84
	assign (segid 3A4 and resid 109 and name CA)	(segid 3A4 and resid 263 and name CB)	13.56	0.85	0.85
40	assign (segid 3A4 and resid 109 and name CA)	(segid 3A4 and resid 264 and name CA)	14.44	0.77	0.77
	assign (segid 3A4 and resid 109 and name CA)	(segid 3A4 and resid 265 and name CA)	17.79	0.76	0.76
	assign (segid 3A4 and resid 109 and name CA)	(segid 3A4 and resid 266 and name CA)	16.89	0.82	0.83
	assign (segid 3A4 and resid 109 and name CA)	(segid 3A4 and resid 267 and name CA)	14.13	0.68	0.69
	assign (segid 3A4 and resid 109 and name CA)	(segid 3A4 and resid 267 and name CB)	12.78	0.67	0.68
45	assign (segid 3A4 and resid 109 and name CA)	(segid 3A4 and resid 268 and name CA)	16.68	0.58	0.59
	assign (segid 3A4 and resid 109 and name CA)	(segid 3A4 and resid 268 and name CB)	17.44	0.53	0.53
	assign (segid 3A4 and resid 109 and name CA)	(segid 3A4 and resid 270 and name CA)	17.56	0.80	0.81
	assign (segid 3A4 and resid 109 and name CA)	(segid 3A4 and resid 270 and name CB)	16.47	0.80	0.80
	assign (segid 3A4 and resid 109 and name CA)	(segid 3A4 and resid 271 and name CA)	16.74	0.94	0.94
50	assign (segid 3A4 and resid 109 and name CA)	(segid 3A4 and resid 271 and name CB)	15.95	0.92	0.93
	assign (segid 3A4 and resid 109 and name CA)	(segid 3A4 and resid 277 and name CB)	17.69	0.99	0.98
	assign (segid 3A4 and resid 109 and name CA)	(segid 3A4 and resid 281 and name CA)	18.30	0.74	0.74
	assign (segid 3A4 and resid 109 and name CA)	(segid 3A4 and resid 281 and name CB)	17.84	0.77	0.77
	assign (segid 3A4 and resid 109 and name CA)	(segid 3A4 and resid 400 and name CA)	16.83	1.05	1.05
55	assign (segid 3A4 and resid 109 and name CA)	(segid 3A4 and resid 400 and name CB)	16.91	1.00	1.00
	assign (segid 3A4 and resid 109 and name CA)	(segid 3A4 and resid 401 and name CA)	16.59	0.91	0.91
	assign (segid 3A4 and resid 109 and name CA)	(segid 3A4 and resid 402 and name CA)	17.52	1.09	1.10
	assign (segid 3A4 and resid 109 and name CA)	(segid 3A4 and resid 403 and name CA)	15.25	1.19	1.19
	assign (segid 3A4 and resid 109 and name CA)	(segid 3A4 and resid 403 and name CB)	15.43	1.23	1.23
60	assign (segid 3A4 and resid 109 and name CA)	(segid 3A4 and resid 404 and name CA)	12.19	1.06	1.06
	assign (segid 3A4 and resid 109 and name CA)	(segid 3A4 and resid 404 and name CB)	12.17	0.99	0.99
	assign (segid 3A4 and resid 109 and name CA)	(segid 3A4 and resid 405 and name CA)	13.43	1.23	1.24
	assign (segid 3A4 and resid 109 and name CA)	(segid 3A4 and resid 405 and name CB)	14.72	1.20	1.19
	assign (segid 3A4 and resid 109 and name CA)	(segid 3A4 and resid 406 and name CA)	14.60	1.28	1.28
65	assign (segid 3A4 and resid 109 and name CA)	(segid 3A4 and resid 407 and name CA)	11.47	1.31	1.31
	assign (segid 3A4 and resid 109 and name CA)	(segid 3A4 and resid 407 and name CB)	11.01	1.39	1.39
	assign (segid 3A4 and resid 109 and name CA)	(segid 3A4 and resid 408 and name CA)	9.32	0.99	0.99
	assign (segid 3A4 and resid 109 and name CA)	(segid 3A4 and resid 408 and name CB)	9.33	0.99	0.99
	assign (segid 3A4 and resid 109 and name CA)	(segid 3A4 and resid 409 and name CA)	12.14	0.73	0.74
70	assign (segid 3A4 and resid 109 and name CA)	(segid 3A4 and resid 409 and name CB)	13.46	0.74	0.74
	assign (segid 3A4 and resid 109 and name CA)	(segid 3A4 and resid 410 and name CA)	12.86	0.80	0.80
	assign (segid 3A4 and resid 109 and name CA)	(segid 3A4 and resid 411 and name CA)	9.75	0.64	0.65
	assign (segid 3A4 and resid 109 and name CA)	(segid 3A4 and resid 411 and name CB)	8.56	0.72	0.73
	assign (segid 3A4 and resid 109 and name CA)	(segid 3A4 and resid 412 and name CA)	9.68	0.59	0.59
75	assign (segid 3A4 and resid 109 and name CA)	(segid 3A4 and resid 413 and name CA)	12.90	0.97	0.97
	assign (segid 3A4 and resid 109 and name CA)	(segid 3A4 and resid 414 and name CA)	12.22	0.87	0.87
	assign (segid 3A4 and resid 109 and name CA)	(segid 3A4 and resid 415 and name CA)	14.23	0.64	0.64
	assign (segid 3A4 and resid 109 and name CA)	(segid 3A4 and resid 415 and name CB)	15.03	0.98	0.99
	assign (segid 3A4 and resid 109 and name CA)	(segid 3A4 and resid 416 and name CA)	15.28	0.54	0.53
80	assign (segid 3A4 and resid 109 and name CA)	(segid 3A4 and resid 417 and name CA)	16.61	1.02	1.02
	assign (segid 3A4 and resid 109 and name CA)	(segid 3A4 and resid 437 and name CA)	16.32	1.08	1.09
	assign (segid 3A4 and resid 109 and name CA)	(segid 3A4 and resid 438 and name CA)	14.49	0.87	0.88
	assign (segid 3A4 and resid 109 and name CA)	(segid 3A4 and resid 439 and name CA)	12.91	0.69	0.69

	assign (segid 3A4 and resid 109 and name CA)	(segid 3A4 and resid 440 and name CA)	11.20	0.66	0.66
	assign (segid 3A4 and resid 109 and name CB)	(segid 3A4 and resid 110 and name C)	5.50	0.03	0.03
	assign (segid 3A4 and resid 109 and name CB)	(segid 3A4 and resid 110 and name CA)	4.57	0.04	0.04
	assign (segid 3A4 and resid 109 and name CB)	(segid 3A4 and resid 110 and name CB)	5.48	0.08	0.08
	assign (segid 3A4 and resid 109 and name CB)	(segid 3A4 and resid 110 and name N)	3.24	0.04	0.05
5	assign (segid 3A4 and resid 109 and name CB)	(segid 3A4 and resid 110 and name O)	6.39	0.14	0.14
	assign (segid 3A4 and resid 109 and name CB)	(segid 3A4 and resid 111 and name C)	6.97	0.08	0.08
	assign (segid 3A4 and resid 109 and name CB)	(segid 3A4 and resid 111 and name CA)	6.83	0.09	0.09
	assign (segid 3A4 and resid 109 and name CB)	(segid 3A4 and resid 111 and name CB)	7.37	0.16	0.17
	assign (segid 3A4 and resid 109 and name CB)	(segid 3A4 and resid 111 and name N)	5.63	0.09	0.09
10	assign (segid 3A4 and resid 109 and name CB)	(segid 3A4 and resid 112 and name C)	7.49	0.19	0.20
	assign (segid 3A4 and resid 109 and name CB)	(segid 3A4 and resid 112 and name CA)	6.74	0.19	0.20
	assign (segid 3A4 and resid 109 and name CB)	(segid 3A4 and resid 112 and name N)	6.19	0.18	0.18
	assign (segid 3A4 and resid 109 and name CB)	(segid 3A4 and resid 119 and name CA)	8.43	1.57	1.57
	assign (segid 3A4 and resid 109 and name CB)	(segid 3A4 and resid 119 and name CB)	7.09	1.49	1.49
15	assign (segid 3A4 and resid 109 and name CB)	(segid 3A4 and resid 120 and name CA)	10.08	1.18	1.18
	assign (segid 3A4 and resid 109 and name CB)	(segid 3A4 and resid 120 and name CB)	11.09	1.18	1.19
	assign (segid 3A4 and resid 109 and name CB)	(segid 3A4 and resid 121 and name CA)	8.50	1.00	1.01
	assign (segid 3A4 and resid 109 and name CB)	(segid 3A4 and resid 121 and name CB)	8.83	0.90	0.89
	assign (segid 3A4 and resid 109 and name CB)	(segid 3A4 and resid 122 and name CA)	11.31	1.09	1.09
20	assign (segid 3A4 and resid 109 and name CB)	(segid 3A4 and resid 122 and name CB)	12.74	1.08	1.08
	assign (segid 3A4 and resid 109 and name CB)	(segid 3A4 and resid 123 and name CA)	11.06	0.99	1.00
	assign (segid 3A4 and resid 109 and name CB)	(segid 3A4 and resid 123 and name CB)	11.59	0.96	0.95
	assign (segid 3A4 and resid 109 and name CB)	(segid 3A4 and resid 124 and name CA)	7.68	1.07	1.08
	assign (segid 3A4 and resid 109 and name CB)	(segid 3A4 and resid 124 and name CB)	6.68	1.09	1.09
25	assign (segid 3A4 and resid 109 and name CB)	(segid 3A4 and resid 125 and name CA)	7.86	1.51	1.50
	assign (segid 3A4 and resid 109 and name CB)	(segid 3A4 and resid 125 and name CB)	7.41	2.01	2.00
	assign (segid 3A4 and resid 109 and name CB)	(segid 3A4 and resid 126 and name CA)	11.07	1.52	1.52
	assign (segid 3A4 and resid 109 and name CB)	(segid 3A4 and resid 127 and name CA)	12.07	0.63	0.63
	assign (segid 3A4 and resid 109 and name CB)	(segid 3A4 and resid 127 and name CB)	11.99	0.91	0.90
30	assign (segid 3A4 and resid 109 and name CB)	(segid 3A4 and resid 128 and name CA)	11.20	0.47	0.47
	assign (segid 3A4 and resid 109 and name CB)	(segid 3A4 and resid 128 and name CB)	10.18	0.51	0.51
	assign (segid 3A4 and resid 109 and name CB)	(segid 3A4 and resid 129 and name CA)	12.14	1.53	1.53
	assign (segid 3A4 and resid 109 and name CB)	(segid 3A4 and resid 129 and name CB)	11.78	1.98	1.98
	assign (segid 3A4 and resid 109 and name CB)	(segid 3A4 and resid 130 and name CA)	15.19	1.00	1.00
35	assign (segid 3A4 and resid 109 and name CB)	(segid 3A4 and resid 130 and name CB)	15.48	0.85	0.85
	assign (segid 3A4 and resid 109 and name CB)	(segid 3A4 and resid 131 and name CA)	15.81	0.39	0.39
	assign (segid 3A4 and resid 109 and name CB)	(segid 3A4 and resid 131 and name CB)	15.26	0.58	0.58
	assign (segid 3A4 and resid 109 and name CB)	(segid 3A4 and resid 132 and name CA)	15.58	0.74	0.74
	assign (segid 3A4 and resid 109 and name CB)	(segid 3A4 and resid 132 and name CB)	14.60	1.01	1.01
40	assign (segid 3A4 and resid 109 and name CB)	(segid 3A4 and resid 259 and name CA)	17.29	0.67	0.67
	assign (segid 3A4 and resid 109 and name CB)	(segid 3A4 and resid 259 and name CB)	17.07	0.68	0.69
	assign (segid 3A4 and resid 109 and name CB)	(segid 3A4 and resid 260 and name CA)	14.88	0.73	0.72
	assign (segid 3A4 and resid 109 and name CB)	(segid 3A4 and resid 260 and name CB)	15.07	0.85	0.84
	assign (segid 3A4 and resid 109 and name CB)	(segid 3A4 and resid 261 and name CA)	16.94	0.73	0.73
45	assign (segid 3A4 and resid 109 and name CB)	(segid 3A4 and resid 262 and name CA)	17.07	0.67	0.68
	assign (segid 3A4 and resid 109 and name CB)	(segid 3A4 and resid 262 and name CB)	17.65	0.70	0.70
	assign (segid 3A4 and resid 109 and name CB)	(segid 3A4 and resid 263 and name CA)	13.40	0.68	0.69
	assign (segid 3A4 and resid 109 and name CB)	(segid 3A4 and resid 263 and name CB)	12.41	0.68	0.68
	assign (segid 3A4 and resid 109 and name CB)	(segid 3A4 and resid 264 and name CA)	13.37	0.71	0.71
50	assign (segid 3A4 and resid 109 and name CB)	(segid 3A4 and resid 264 and name CB)	13.37	0.71	0.71
	assign (segid 3A4 and resid 109 and name CB)	(segid 3A4 and resid 265 and name CA)	16.64	0.70	0.70
	assign (segid 3A4 and resid 109 and name CB)	(segid 3A4 and resid 265 and name CB)	16.64	0.76	0.76
	assign (segid 3A4 and resid 109 and name CB)	(segid 3A4 and resid 266 and name CA)	15.60	0.66	0.65
	assign (segid 3A4 and resid 109 and name CB)	(segid 3A4 and resid 267 and name CA)	12.90	0.66	0.65
	assign (segid 3A4 and resid 109 and name CB)	(segid 3A4 and resid 267 and name CB)	11.58	0.66	0.67
	assign (segid 3A4 and resid 109 and name CB)	(segid 3A4 and resid 268 and name CA)	15.57	0.62	0.62
55	assign (segid 3A4 and resid 109 and name CB)	(segid 3A4 and resid 268 and name CB)	16.36	0.59	0.59
	assign (segid 3A4 and resid 109 and name CB)	(segid 3A4 and resid 269 and name CA)	18.05	0.67	0.68
	assign (segid 3A4 and resid 109 and name CB)	(segid 3A4 and resid 270 and name CA)	16.30	0.79	0.80
	assign (segid 3A4 and resid 109 and name CB)	(segid 3A4 and resid 270 and name CB)	15.19	0.80	0.79
	assign (segid 3A4 and resid 109 and name CB)	(segid 3A4 and resid 271 and name CA)	15.65	0.93	0.93
60	assign (segid 3A4 and resid 109 and name CB)	(segid 3A4 and resid 271 and name CB)	14.91	0.94	0.94
	assign (segid 3A4 and resid 109 and name CB)	(segid 3A4 and resid 277 and name CA)	17.31	0.94	0.94
	assign (segid 3A4 and resid 109 and name CB)	(segid 3A4 and resid 277 and name CB)	16.49	1.00	0.99
	assign (segid 3A4 and resid 109 and name CB)	(segid 3A4 and resid 280 and name CA)	18.59	0.77	0.78
	assign (segid 3A4 and resid 109 and name CB)	(segid 3A4 and resid 280 and name CB)	17.61	0.81	0.81
65	assign (segid 3A4 and resid 109 and name CB)	(segid 3A4 and resid 281 and name CA)	17.12	0.93	0.93
	assign (segid 3A4 and resid 109 and name CB)	(segid 3A4 and resid 281 and name CB)	16.70	0.94	0.93
	assign (segid 3A4 and resid 109 and name CB)	(segid 3A4 and resid 399 and name CA)	18.91	1.10	1.09
	assign (segid 3A4 and resid 109 and name CB)	(segid 3A4 and resid 400 and name CA)	15.78	0.94	0.93
	assign (segid 3A4 and resid 109 and name CB)	(segid 3A4 and resid 400 and name CB)	15.91	0.85	0.85
70	assign (segid 3A4 and resid 109 and name CB)	(segid 3A4 and resid 401 and name CA)	15.37	0.80	0.81
	assign (segid 3A4 and resid 109 and name CB)	(segid 3A4 and resid 402 and name CA)	16.26	1.08	1.08
	assign (segid 3A4 and resid 109 and name CB)	(segid 3A4 and resid 402 and name CB)	17.63	1.14	1.15
	assign (segid 3A4 and resid 109 and name CB)	(segid 3A4 and resid 403 and name CA)	14.10	1.20	1.21
	assign (segid 3A4 and resid 109 and name CB)	(segid 3A4 and resid 403 and name CB)	14.36	1.23	1.23
75	assign (segid 3A4 and resid 109 and name CB)	(segid 3A4 and resid 404 and name CA)	11.00	0.99	1.00
	assign (segid 3A4 and resid 109 and name CB)	(segid 3A4 and resid 404 and name CB)	11.00	0.86	0.85
	assign (segid 3A4 and resid 109 and name CB)	(segid 3A4 and resid 405 and name CA)	12.12	1.23	1.24
	assign (segid 3A4 and resid 109 and name CB)	(segid 3A4 and resid 405 and name CB)	13.39	1.19	1.19
	assign (segid 3A4 and resid 109 and name CB)	(segid 3A4 and resid 406 and name CA)	13.36	1.39	1.39
80	assign (segid 3A4 and resid 109 and name CB)	(segid 3A4 and resid 407 and name CA)	10.35	1.47	1.46
	assign (segid 3A4 and resid 109 and name CB)	(segid 3A4 and resid 407 and name CB)	9.95	1.54	1.54
	assign (segid 3A4 and resid 109 and name CB)	(segid 3A4 and resid 408 and name CA)	8.09	1.05	1.05

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	assign (segid 3A4 and resid 10 and name CA) (segid 3A4 and resid 13 and name CB)	4.56	0.34	0.34
	assign (segid 3A4 and resid 10 and name CA) (segid 3A4 and resid 13 and name N)	4.61	0.20	0.20
	assign (segid 3A4 and resid 10 and name CA) (segid 3A4 and resid 19 and name CA)	10.37	1.40	1.40
	assign (segid 3A4 and resid 10 and name CA) (segid 3A4 and resid 19 and name CB)	11.54	1.49	1.49
5	assign (segid 3A4 and resid 10 and name CA) (segid 3A4 and resid 20 and name CA)	11.55	0.92	0.91
	assign (segid 3A4 and resid 10 and name CA) (segid 3A4 and resid 20 and name CB)	12.94	0.91	0.91
	assign (segid 3A4 and resid 10 and name CA) (segid 3A4 and resid 21 and name CA)	11.16	1.03	1.04
	assign (segid 3A4 and resid 10 and name CA) (segid 3A4 and resid 21 and name CB)	10.14	1.07	1.06
	assign (segid 3A4 and resid 10 and name CA) (segid 3A4 and resid 22 and name CA)	12.73	1.34	1.34
10	assign (segid 3A4 and resid 10 and name CA) (segid 3A4 and resid 23 and name CA)	11.85	1.50	1.50
	assign (segid 3A4 and resid 10 and name CA) (segid 3A4 and resid 23 and name CB)	10.72	1.65	1.65
	assign (segid 3A4 and resid 10 and name CA) (segid 3A4 and resid 24 and name CA)	14.77	1.57	1.58
	assign (segid 3A4 and resid 10 and name CA) (segid 3A4 and resid 24 and name CB)	15.70	1.50	1.50
	assign (segid 3A4 and resid 10 and name CA) (segid 3A4 and resid 25 and name CA)	15.23	1.95	1.94
15	assign (segid 3A4 and resid 10 and name CA) (segid 3A4 and resid 29 and name CA)	16.74	1.48	1.48
	assign (segid 3A4 and resid 10 and name CA) (segid 3A4 and resid 30 and name CA)	14.65	1.78	1.78
	assign (segid 3A4 and resid 10 and name CA) (segid 3A4 and resid 314 and name CA)	16.51	1.62	1.62
	assign (segid 3A4 and resid 10 and name CA) (segid 3A4 and resid 314 and name CB)	17.09	1.58	1.58
	assign (segid 3A4 and resid 10 and name CA) (segid 3A4 and resid 315 and name CA)	15.26	1.82	1.81
20	assign (segid 3A4 and resid 10 and name CA) (segid 3A4 and resid 315 and name CB)	16.28	1.83	1.84
	assign (segid 3A4 and resid 10 and name CA) (segid 3A4 and resid 316 and name CA)	15.00	2.15	2.14
	assign (segid 3A4 and resid 10 and name CA) (segid 3A4 and resid 317 and name CA)	14.24	1.82	1.82
	assign (segid 3A4 and resid 10 and name CA) (segid 3A4 and resid 31 and name CA)	13.08	1.41	1.42
	assign (segid 3A4 and resid 10 and name CA) (segid 3A4 and resid 31 and name CB)	14.07	1.27	1.26
25	assign (segid 3A4 and resid 10 and name CA) (segid 3A4 and resid 32 and name CA)	9.97	1.36	1.35
	assign (segid 3A4 and resid 10 and name CA) (segid 3A4 and resid 32 and name CB)	8.71	1.49	1.49
	assign (segid 3A4 and resid 10 and name CA) (segid 3A4 and resid 33 and name CA)	10.65	0.90	0.91
	assign (segid 3A4 and resid 10 and name CA) (segid 3A4 and resid 33 and name CB)	11.90	0.86	0.86
	assign (segid 3A4 and resid 10 and name CA) (segid 3A4 and resid 343 and name CA)	15.19	1.57	1.58
30	assign (segid 3A4 and resid 10 and name CA) (segid 3A4 and resid 343 and name CB)	15.77	1.40	1.40
	assign (segid 3A4 and resid 10 and name CA) (segid 3A4 and resid 344 and name CA)	12.55	1.78	1.78
	assign (segid 3A4 and resid 10 and name CA) (segid 3A4 and resid 344 and name CB)	11.69	1.91	1.91
	assign (segid 3A4 and resid 10 and name CA) (segid 3A4 and resid 345 and name CA)	12.09	1.46	1.46
	assign (segid 3A4 and resid 10 and name CA) (segid 3A4 and resid 345 and name CB)	13.40	1.36	1.35
35	assign (segid 3A4 and resid 10 and name CA) (segid 3A4 and resid 346 and name CA)	9.45	1.60	1.60
	assign (segid 3A4 and resid 10 and name CA) (segid 3A4 and resid 346 and name CB)	8.11	1.58	1.57
	assign (segid 3A4 and resid 10 and name CA) (segid 3A4 and resid 347 and name CA)	11.81	1.38	1.38
	assign (segid 3A4 and resid 10 and name CA) (segid 3A4 and resid 347 and name CB)	12.98	1.50	1.50
	assign (segid 3A4 and resid 10 and name CA) (segid 3A4 and resid 348 and name CA)	10.05	1.52	1.52
40	assign (segid 3A4 and resid 10 and name CA) (segid 3A4 and resid 349 and name CA)	8.10	1.49	1.50
	assign (segid 3A4 and resid 10 and name CA) (segid 3A4 and resid 349 and name CB)	7.33	1.47	1.47
	assign (segid 3A4 and resid 10 and name CA) (segid 3A4 and resid 34 and name CA)	8.54	1.19	1.18
	assign (segid 3A4 and resid 10 and name CA) (segid 3A4 and resid 34 and name CB)	7.54	1.35	1.34
	assign (segid 3A4 and resid 10 and name CA) (segid 3A4 and resid 350 and name CA)	11.32	1.37	1.37
45	assign (segid 3A4 and resid 10 and name CA) (segid 3A4 and resid 350 and name CB)	12.27	1.26	1.26
	assign (segid 3A4 and resid 10 and name CA) (segid 3A4 and resid 351 and name CA)	12.91	1.41	1.40
	assign (segid 3A4 and resid 10 and name CA) (segid 3A4 and resid 352 and name CA)	11.07	1.78	1.79
	assign (segid 3A4 and resid 10 and name CA) (segid 3A4 and resid 352 and name CB)	10.01	1.83	1.82
	assign (segid 3A4 and resid 10 and name CA) (segid 3A4 and resid 353 and name CA)	11.76	1.92	1.93
50	assign (segid 3A4 and resid 10 and name CA) (segid 3A4 and resid 353 and name CB)	12.30	1.91	1.91
	assign (segid 3A4 and resid 10 and name CA) (segid 3A4 and resid 354 and name CA)	13.95	2.14	2.13
	assign (segid 3A4 and resid 10 and name CA) (segid 3A4 and resid 354 and name CB)	13.73	2.26	2.25
	assign (segid 3A4 and resid 10 and name CA) (segid 3A4 and resid 356 and name CA)	16.51	1.84	1.85
	assign (segid 3A4 and resid 10 and name CA) (segid 3A4 and resid 357 and name CA)	16.38	1.89	1.90
55	assign (segid 3A4 and resid 10 and name CA) (segid 3A4 and resid 35 and name CA)	11.19	1.33	1.33
	assign (segid 3A4 and resid 10 and name CA) (segid 3A4 and resid 360 and name CA)	14.52	2.00	2.00
	assign (segid 3A4 and resid 10 and name CA) (segid 3A4 and resid 360 and name CB)	13.40	2.01	2.01
	assign (segid 3A4 and resid 10 and name CA) (segid 3A4 and resid 361 and name CA)	14.07	1.93	1.93
	assign (segid 3A4 and resid 10 and name CA) (segid 3A4 and resid 361 and name CB)	13.51	1.98	1.98
60	assign (segid 3A4 and resid 10 and name CA) (segid 3A4 and resid 36 and name CA)	13.78	1.48	1.48
	assign (segid 3A4 and resid 10 and name CA) (segid 3A4 and resid 37 and name CA)	16.31	1.16	1.16
	assign (segid 3A4 and resid 10 and name CA) (segid 3A4 and resid 37 and name CB)	16.61	1.06	1.05
	assign (segid 3A4 and resid 10 and name CA) (segid 3A4 and resid 382 and name CA)	16.93	1.40	1.39
	assign (segid 3A4 and resid 10 and name CA) (segid 3A4 and resid 382 and name CB)	16.14	1.31	1.31
65	assign (segid 3A4 and resid 10 and name CA) (segid 3A4 and resid 38 and name CA)	15.18	1.07	1.07
	assign (segid 3A4 and resid 10 and name CA) (segid 3A4 and resid 38 and name CB)	14.15	1.11	1.11
	assign (segid 3A4 and resid 10 and name CA) (segid 3A4 and resid 39 and name CA)	14.69	1.11	1.11
	assign (segid 3A4 and resid 10 and name CA) (segid 3A4 and resid 39 and name CB)	13.79	1.18	1.17
	assign (segid 3A4 and resid 10 and name CA) (segid 3A4 and resid 429 and name CA)	14.51	2.46	2.45
70	assign (segid 3A4 and resid 10 and name CA) (segid 3A4 and resid 42 and name CA)	17.14	0.92	0.91
	assign (segid 3A4 and resid 10 and name CA) (segid 3A4 and resid 430 and name CA)	13.90	1.90	1.90
	assign (segid 3A4 and resid 10 and name CA) (segid 3A4 and resid 433 and name CA)	15.20	2.23	2.23
	assign (segid 3A4 and resid 10 and name CB) (segid 3A4 and resid 11 and name C)	5.49	0.07	0.07
75	assign (segid 3A4 and resid 10 and name CB) (segid 3A4 and resid 11 and name CA)	4.55	0.05	0.05
	assign (segid 3A4 and resid 10 and name CB) (segid 3A4 and resid 11 and name CB)	5.43	0.04	0.05
	assign (segid 3A4 and resid 10 and name CB) (segid 3A4 and resid 11 and name N)	3.23	0.05	0.06
	assign (segid 3A4 and resid 10 and name CB) (segid 3A4 and resid 11 and name O)	6.41	0.16	0.17
	assign (segid 3A4 and resid 10 and name CB) (segid 3A4 and resid 12 and name C)	6.89	0.11	0.11
80	assign (segid 3A4 and resid 10 and name CB) (segid 3A4 and resid 12 and name CA)	6.81	0.07	0.06
	assign (segid 3A4 and resid 10 and name CB) (segid 3A4 and resid 12 and name CB)	7.24	0.08	0.09
	assign (segid 3A4 and resid 10 and name CB) (segid 3A4 and resid 12 and name N)	5.62	0.06	0.07
	assign (segid 3A4 and resid 10 and name CB) (segid 3A4 and resid 13 and name C)	6.86	0.36	0.35
	assign (segid 3A4 and resid 10 and name CB) (segid 3A4 and resid 13 and name CA)	6.41	0.22	0.21

	assign (segid 3A4 and resid 10 and name CB) (segid 3A4 and resid 13 and name CB)	5.63	0.24	0.24
	assign (segid 3A4 and resid 10 and name CB) (segid 3A4 and resid 13 and name N)	5.96	0.12	0.13
	assign (segid 3A4 and resid 10 and name CB) (segid 3A4 and resid 19 and name CA)	10.71	1.24	1.24
	assign (segid 3A4 and resid 10 and name CB) (segid 3A4 and resid 19 and name CB)	11.84	1.30	1.29
	assign (segid 3A4 and resid 10 and name CB) (segid 3A4 and resid 20 and name CA)	11.72	0.97	0.98
5	assign (segid 3A4 and resid 10 and name CB) (segid 3A4 and resid 20 and name CB)	13.05	0.97	0.96
	assign (segid 3A4 and resid 10 and name CB) (segid 3A4 and resid 21 and name CA)	11.47	1.19	1.19
	assign (segid 3A4 and resid 10 and name CB) (segid 3A4 and resid 21 and name CB)	10.57	1.22	1.21
	assign (segid 3A4 and resid 10 and name CB) (segid 3A4 and resid 22 and name CA)	12.90	1.55	1.55
	assign (segid 3A4 and resid 10 and name CB) (segid 3A4 and resid 23 and name CA)	12.01	1.67	1.67
10	assign (segid 3A4 and resid 10 and name CB) (segid 3A4 and resid 23 and name CB)	10.84	1.81	1.80
	assign (segid 3A4 and resid 10 and name CB) (segid 3A4 and resid 24 and name CA)	14.85	1.70	1.71
	assign (segid 3A4 and resid 10 and name CB) (segid 3A4 and resid 24 and name CB)	15.84	1.61	1.61
	assign (segid 3A4 and resid 10 and name CB) (segid 3A4 and resid 25 and name CA)	15.19	2.01	2.01
	assign (segid 3A4 and resid 10 and name CB) (segid 3A4 and resid 29 and name CA)	16.62	1.72	1.73
15	assign (segid 3A4 and resid 10 and name CB) (segid 3A4 and resid 30 and name CA)	14.40	2.11	2.11
	assign (segid 3A4 and resid 10 and name CB) (segid 3A4 and resid 315 and name CA)	14.67	2.24	2.25
	assign (segid 3A4 and resid 10 and name CB) (segid 3A4 and resid 315 and name CB)	15.76	2.22	2.22
	assign (segid 3A4 and resid 10 and name CB) (segid 3A4 and resid 316 and name CA)	14.27	2.56	2.57
	assign (segid 3A4 and resid 10 and name CB) (segid 3A4 and resid 317 and name CA)	13.36	2.39	2.39
20	assign (segid 3A4 and resid 10 and name CB) (segid 3A4 and resid 31 and name CA)	12.91	1.72	1.73
	assign (segid 3A4 and resid 10 and name CB) (segid 3A4 and resid 31 and name CB)	13.90	1.56	1.57
	assign (segid 3A4 and resid 10 and name CB) (segid 3A4 and resid 32 and name CA)	9.71	1.70	1.70
	assign (segid 3A4 and resid 10 and name CB) (segid 3A4 and resid 32 and name CB)	8.51	1.81	1.81
	assign (segid 3A4 and resid 10 and name CB) (segid 3A4 and resid 33 and name CA)	10.36	1.25	1.26
25	assign (segid 3A4 and resid 10 and name CB) (segid 3A4 and resid 33 and name CB)	11.53	1.27	1.27
	assign (segid 3A4 and resid 10 and name CB) (segid 3A4 and resid 343 and name CA)	14.69	2.04	2.03
	assign (segid 3A4 and resid 10 and name CB) (segid 3A4 and resid 343 and name CB)	15.28	1.88	1.88
	assign (segid 3A4 and resid 10 and name CB) (segid 3A4 and resid 344 and name CA)	11.89	2.29	2.29
30	assign (segid 3A4 and resid 10 and name CB) (segid 3A4 and resid 344 and name CB)	11.04	2.39	2.40
	assign (segid 3A4 and resid 10 and name CB) (segid 3A4 and resid 345 and name CA)	11.36	2.03	2.03
	assign (segid 3A4 and resid 10 and name CB) (segid 3A4 and resid 345 and name CB)	12.65	1.95	1.95
	assign (segid 3A4 and resid 10 and name CB) (segid 3A4 and resid 346 and name CA)	8.64	2.18	2.17
	assign (segid 3A4 and resid 10 and name CB) (segid 3A4 and resid 346 and name CB)	7.37	2.11	2.10
	assign (segid 3A4 and resid 10 and name CB) (segid 3A4 and resid 347 and name CA)	10.94	2.06	2.05
35	assign (segid 3A4 and resid 10 and name CB) (segid 3A4 and resid 347 and name CB)	12.06	2.18	2.19
	assign (segid 3A4 and resid 10 and name CB) (segid 3A4 and resid 348 and name CA)	9.22	2.19	2.20
	assign (segid 3A4 and resid 10 and name CB) (segid 3A4 and resid 349 and name CA)	7.51	2.11	2.12
	assign (segid 3A4 and resid 10 and name CB) (segid 3A4 and resid 349 and name CB)	6.81	2.02	2.03
	assign (segid 3A4 and resid 10 and name CB) (segid 3A4 and resid 34 and name CA)	8.38	1.44	1.44
40	assign (segid 3A4 and resid 10 and name CB) (segid 3A4 and resid 34 and name CB)	7.58	1.49	1.48
	assign (segid 3A4 and resid 10 and name CB) (segid 3A4 and resid 350 and name CA)	10.78	1.85	1.85
	assign (segid 3A4 and resid 10 and name CB) (segid 3A4 and resid 350 and name CB)	11.66	1.77	1.77
	assign (segid 3A4 and resid 10 and name CB) (segid 3A4 and resid 351 and name CA)	12.32	1.96	1.96
	assign (segid 3A4 and resid 10 and name CB) (segid 3A4 and resid 352 and name CA)	10.76	2.18	2.19
45	assign (segid 3A4 and resid 10 and name CB) (segid 3A4 and resid 352 and name CB)	9.69	2.25	2.25
	assign (segid 3A4 and resid 10 and name CB) (segid 3A4 and resid 353 and name CA)	11.69	2.11	2.10
	assign (segid 3A4 and resid 10 and name CB) (segid 3A4 and resid 353 and name CB)	12.17	2.08	2.08
	assign (segid 3A4 and resid 10 and name CB) (segid 3A4 and resid 354 and name CA)	14.09	2.16	2.16
	assign (segid 3A4 and resid 10 and name CB) (segid 3A4 and resid 354 and name CB)	14.00	2.23	2.22
50	assign (segid 3A4 and resid 10 and name CB) (segid 3A4 and resid 356 and name CB)	16.28	2.04	2.03
	assign (segid 3A4 and resid 10 and name CB) (segid 3A4 and resid 357 and name CB)	16.14	2.18	2.18
	assign (segid 3A4 and resid 10 and name CB) (segid 3A4 and resid 35 and name CA)	11.10	1.47	1.46
	assign (segid 3A4 and resid 10 and name CB) (segid 3A4 and resid 360 and name CA)	14.42	2.28	2.28
	assign (segid 3A4 and resid 10 and name CB) (segid 3A4 and resid 360 and name CB)	13.32	2.29	2.29
55	assign (segid 3A4 and resid 10 and name CB) (segid 3A4 and resid 361 and name CA)	14.01	2.21	2.21
	assign (segid 3A4 and resid 10 and name CB) (segid 3A4 and resid 361 and name CB)	13.56	2.21	2.21
	assign (segid 3A4 and resid 10 and name CB) (segid 3A4 and resid 36 and name CA)	13.43	1.76	1.76
	assign (segid 3A4 and resid 10 and name CB) (segid 3A4 and resid 37 and name CA)	16.07	1.34	1.33
60	assign (segid 3A4 and resid 10 and name CB) (segid 3A4 and resid 37 and name CB)	16.46	1.11	1.11
	assign (segid 3A4 and resid 10 and name CB) (segid 3A4 and resid 382 and name CB)	15.31	1.92	1.93
	assign (segid 3A4 and resid 10 and name CB) (segid 3A4 and resid 38 and name CA)	14.92	1.27	1.27
	assign (segid 3A4 and resid 10 and name CB) (segid 3A4 and resid 38 and name CB)	13.97	1.27	1.26
	assign (segid 3A4 and resid 10 and name CB) (segid 3A4 and resid 39 and name CA)	14.16	1.54	1.55
	assign (segid 3A4 and resid 10 and name CB) (segid 3A4 and resid 39 and name CB)	13.21	1.66	1.66
65	assign (segid 3A4 and resid 10 and name CB) (segid 3A4 and resid 429 and name CA)	13.87	2.44	2.44
	assign (segid 3A4 and resid 10 and name CB) (segid 3A4 and resid 430 and name CA)	13.13	2.02	2.02
	assign (segid 3A4 and resid 10 and name CB) (segid 3A4 and resid 431 and name CA)	14.31	2.28	2.28
	assign (segid 3A4 and resid 10 and name CB) (segid 3A4 and resid 433 and name CA)	14.41	2.48	2.49
	assign (segid 3A4 and resid 10 and name CB) (segid 3A4 and resid 10 and name C)	2.45	0.04	0.04
70	assign (segid 3A4 and resid 10 and name N) (segid 3A4 and resid 10 and name CA)	1.46	0.00	0.01
	assign (segid 3A4 and resid 10 and name N) (segid 3A4 and resid 10 and name CB)	2.48	0.01	0.01
	assign (segid 3A4 and resid 10 and name N) (segid 3A4 and resid 10 and name O)	3.52	0.03	0.04
	assign (segid 3A4 and resid 10 and name N) (segid 3A4 and resid 11 and name C)	4.69	0.09	0.10
	assign (segid 3A4 and resid 10 and name N) (segid 3A4 and resid 11 and name CA)	4.18	0.09	0.09
75	assign (segid 3A4 and resid 10 and name N) (segid 3A4 and resid 11 and name CB)	4.92	0.09	0.09
	assign (segid 3A4 and resid 10 and name N) (segid 3A4 and resid 11 and name N)	2.78	0.10	0.11
	assign (segid 3A4 and resid 10 and name N) (segid 3A4 and resid 11 and name O)	5.82	0.14	0.14
	assign (segid 3A4 and resid 10 and name N) (segid 3A4 and resid 12 and name CA)	5.75	0.24	0.23
	assign (segid 3A4 and resid 10 and name N) (segid 3A4 and resid 12 and name CB)	5.33	0.09	0.09
80	assign (segid 3A4 and resid 10 and name N) (segid 3A4 and resid 12 and name N)	5.36	0.13	0.13
	assign (segid 3A4 and resid 10 and name N) (segid 3A4 and resid 12 and name O)	4.29	0.10	0.09
	assign (segid 3A4 and resid 10 and name N) (segid 3A4 and resid 12 and name O)	6.94	0.24	0.25

assign (segid 3A4 and resid 10 and name N) (segid 3A4 and resid 13 and name CA) 5.86 0.44 0.44
assign (segid 3A4 and resid 10 and name N) (segid 3A4 and resid 13 and name CB) 5.34 0.49 0.49
assign (segid 3A4 and resid 10 and name N) (segid 3A4 and resid 13 and name N) 5.01 0.35 0.35
assign (segid 3A4 and resid 10 and name O) (segid 3A4 and resid 10 and name CB) 3.22 0.03 0.03
5 assign (segid 3A4 and resid 10 and name O) (segid 3A4 and resid 11 and name C) 3.04 0.13 0.14
assign (segid 3A4 and resid 10 and name O) (segid 3A4 and resid 11 and name CA) 2.75 0.04 0.04
assign (segid 3A4 and resid 10 and name O) (segid 3A4 and resid 11 and name CB) 4.22 0.03 0.04
assign (segid 3A4 and resid 10 and name O) (segid 3A4 and resid 11 and name N) 2.23 0.02 0.02
assign (segid 3A4 and resid 10 and name O) (segid 3A4 and resid 11 and name O) 3.62 0.25 0.24
10 assign (segid 3A4 and resid 10 and name O) (segid 3A4 and resid 12 and name C) 4.14 0.18 0.18
assign (segid 3A4 and resid 10 and name O) (segid 3A4 and resid 12 and name CA) 4.41 0.23 0.24
assign (segid 3A4 and resid 10 and name O) (segid 3A4 and resid 12 and name CB) 5.32 0.26 0.26
assign (segid 3A4 and resid 10 and name O) (segid 3A4 and resid 12 and name N) 3.44 0.22 0.21
assign (segid 3A4 and resid 10 and name O) (segid 3A4 and resid 12 and name O) 5.07 0.19 0.18
15 assign (segid 3A4 and resid 10 and name O) (segid 3A4 and resid 13 and name C) 3.90 0.28 0.29
assign (segid 3A4 and resid 10 and name O) (segid 3A4 and resid 13 and name CA) 3.74 0.11 0.11
assign (segid 3A4 and resid 10 and name O) (segid 3A4 and resid 13 and name CB) 3.55 0.16 0.15
assign (segid 3A4 and resid 10 and name O) (segid 3A4 and resid 13 and name N) 3.30 0.18 0.18
assign (segid 3A4 and resid 10 and name O) (segid 3A4 and resid 13 and name O) 5.06 0.25 0.25
20 assign (segid 3A4 and resid 10 and name O) (segid 3A4 and resid 34 and name CB) 6.18 1.13 1.14
assign (segid 3A4 and resid 110 and name CB) (segid 3A4 and resid 110 and name CB) 2.48 0.03 0.03
assign (segid 3A4 and resid 110 and name C) (segid 3A4 and resid 110 and name O) 1.23 0.00 0.00
assign (segid 3A4 and resid 110 and name C) (segid 3A4 and resid 111 and name C) 3.20 0.10 0.09
assign (segid 3A4 and resid 110 and name C) (segid 3A4 and resid 111 and name CA) 2.44 0.01 0.02
25 assign (segid 3A4 and resid 110 and name C) (segid 3A4 and resid 111 and name CB) 3.65 0.03 0.04
assign (segid 3A4 and resid 110 and name C) (segid 3A4 and resid 111 and name N) 1.33 0.01 0.00
assign (segid 3A4 and resid 110 and name C) (segid 3A4 and resid 111 and name O) 4.32 0.10 0.09
assign (segid 3A4 and resid 110 and name C) (segid 3A4 and resid 112 and name C) 4.82 0.21 0.21
assign (segid 3A4 and resid 110 and name C) (segid 3A4 and resid 112 and name CA) 4.47 0.21 0.21
30 assign (segid 3A4 and resid 110 and name C) (segid 3A4 and resid 112 and name N) 3.18 0.19 0.18
assign (segid 3A4 and resid 110 and name C) (segid 3A4 and resid 112 and name O) 5.43 0.71 0.71
assign (segid 3A4 and resid 110 and name CA) (segid 3A4 and resid 110 and name C) 1.52 0.01 0.01
assign (segid 3A4 and resid 110 and name CA) (segid 3A4 and resid 110 and name CB) 1.52 0.01 0.01
35 assign (segid 3A4 and resid 110 and name CA) (segid 3A4 and resid 110 and name O) 2.40 0.02 0.01
assign (segid 3A4 and resid 110 and name CA) (segid 3A4 and resid 111 and name C) 4.56 0.09 0.09
assign (segid 3A4 and resid 110 and name CA) (segid 3A4 and resid 111 and name CA) 3.81 0.02 0.01
assign (segid 3A4 and resid 110 and name CA) (segid 3A4 and resid 111 and name CB) 4.79 0.05 0.05
40 assign (segid 3A4 and resid 110 and name CA) (segid 3A4 and resid 111 and name N) 2.43 0.01 0.01
assign (segid 3A4 and resid 110 and name CA) (segid 3A4 and resid 111 and name O) 5.72 0.07 0.07
assign (segid 3A4 and resid 110 and name CA) (segid 3A4 and resid 112 and name C) 5.85 0.28 0.28
45 assign (segid 3A4 and resid 110 and name CA) (segid 3A4 and resid 112 and name CA) 5.49 0.23 0.24
assign (segid 3A4 and resid 110 and name CA) (segid 3A4 and resid 112 and name N) 4.31 0.19 0.19
assign (segid 3A4 and resid 110 and name CA) (segid 3A4 and resid 112 and name O) 6.43 0.78 0.77
assign (segid 3A4 and resid 110 and name CA) (segid 3A4 and resid 119 and name CA) 10.57 1.03 1.03
50 assign (segid 3A4 and resid 110 and name CA) (segid 3A4 and resid 119 and name CB) 9.36 0.93 0.93
assign (segid 3A4 and resid 110 and name CA) (segid 3A4 and resid 120 and name CA) 13.12 0.78 0.77
assign (segid 3A4 and resid 110 and name CA) (segid 3A4 and resid 120 and name CB) 14.11 0.66 0.66
assign (segid 3A4 and resid 110 and name CA) (segid 3A4 and resid 121 and name CA) 12.19 0.98 0.98
55 assign (segid 3A4 and resid 110 and name CA) (segid 3A4 and resid 121 and name CB) 12.49 1.01 1.02
assign (segid 3A4 and resid 110 and name CA) (segid 3A4 and resid 122 and name CA) 15.22 1.03 1.03
assign (segid 3A4 and resid 110 and name CA) (segid 3A4 and resid 122 and name CB) 16.59 1.02 1.01
assign (segid 3A4 and resid 110 and name CA) (segid 3A4 and resid 123 and name CA) 14.65 0.83 0.82
60 assign (segid 3A4 and resid 110 and name CA) (segid 3A4 and resid 123 and name CB) 14.94 0.78 0.78
assign (segid 3A4 and resid 110 and name CA) (segid 3A4 and resid 124 and name CA) 11.21 0.94 0.94
assign (segid 3A4 and resid 110 and name CA) (segid 3A4 and resid 124 and name CB) 10.07 0.81 0.81
65 assign (segid 3A4 and resid 110 and name CA) (segid 3A4 and resid 125 and name CA) 11.88 1.56 1.57
assign (segid 3A4 and resid 110 and name CA) (segid 3A4 and resid 125 and name CB) 11.51 2.09 2.08
assign (segid 3A4 and resid 110 and name CA) (segid 3A4 and resid 126 and name CA) 15.10 1.45 1.45
assign (segid 3A4 and resid 110 and name CA) (segid 3A4 and resid 126 and name CB) 15.82 0.62 0.62
70 assign (segid 3A4 and resid 110 and name CA) (segid 3A4 and resid 127 and name CA) 15.63 0.99 1.00
assign (segid 3A4 and resid 110 and name CA) (segid 3A4 and resid 127 and name CB) 14.70 0.70 0.69
assign (segid 3A4 and resid 110 and name CA) (segid 3A4 and resid 128 and name CA) 13.63 0.76 0.76
75 assign (segid 3A4 and resid 110 and name CA) (segid 3A4 and resid 128 and name CB) 15.70 1.73 1.72
assign (segid 3A4 and resid 110 and name CA) (segid 3A4 and resid 129 and name CA) 15.45 2.16 2.16
assign (segid 3A4 and resid 110 and name CA) (segid 3A4 and resid 132 and name CA) 18.53 1.20 1.19
80 assign (segid 3A4 and resid 110 and name CA) (segid 3A4 and resid 132 and name CB) 17.53 1.50 1.49
assign (segid 3A4 and resid 110 and name CA) (segid 3A4 and resid 260 and name CA) 19.02 0.59 0.59
assign (segid 3A4 and resid 110 and name CA) (segid 3A4 and resid 263 and name CA) 17.39 0.53 0.52
assign (segid 3A4 and resid 110 and name CA) (segid 3A4 and resid 263 and name CB) 16.43 0.52 0.51
70 assign (segid 3A4 and resid 110 and name CA) (segid 3A4 and resid 264 and name CA) 17.34 0.65 0.64
assign (segid 3A4 and resid 110 and name CA) (segid 3A4 and resid 267 and name CA) 16.23 0.89 0.88
assign (segid 3A4 and resid 110 and name CA) (segid 3A4 and resid 267 and name CB) 15.01 0.87 0.87
assign (segid 3A4 and resid 110 and name CA) (segid 3A4 and resid 271 and name CB) 17.38 1.44 1.44
75 assign (segid 3A4 and resid 110 and name CA) (segid 3A4 and resid 400 and name CA) 19.01 0.66 0.66
assign (segid 3A4 and resid 110 and name CA) (segid 3A4 and resid 401 and name CA) 18.79 0.52 0.52
80 assign (segid 3A4 and resid 110 and name CA) (segid 3A4 and resid 403 and name CA) 16.64 0.69 0.69
assign (segid 3A4 and resid 110 and name CA) (segid 3A4 and resid 403 and name CB) 16.88 0.79 0.79
assign (segid 3A4 and resid 110 and name CA) (segid 3A4 and resid 404 and name CA) 13.97 0.52 0.52
assign (segid 3A4 and resid 110 and name CA) (segid 3A4 and resid 404 and name CB) 14.26 0.50 0.50
assign (segid 3A4 and resid 110 and name CA) (segid 3A4 and resid 405 and name CA) 14.90 0.72 0.72
assign (segid 3A4 and resid 110 and name CA) (segid 3A4 and resid 405 and name CB) 16.25 0.72 0.73
assign (segid 3A4 and resid 110 and name CA) (segid 3A4 and resid 406 and name CA) 15.34 0.68 0.69
assign (segid 3A4 and resid 110 and name CA) (segid 3A4 and resid 407 and name CA) 11.98 0.65 0.66

	assign (segid 3A4 and resid 110 and name CA) (segid 3A4 and resid 407 and name CB)	11.69	0.72	0.73
	assign (segid 3A4 and resid 110 and name CA) (segid 3A4 and resid 408 and name CA)	10.14	0.62	0.62
	assign (segid 3A4 and resid 110 and name CA) (segid 3A4 and resid 408 and name CB)	10.58	0.80	0.79
	assign (segid 3A4 and resid 110 and name CA) (segid 3A4 and resid 409 and name CA)	12.31	0.65	0.66
	assign (segid 3A4 and resid 110 and name CA) (segid 3A4 and resid 409 and name CB)	13.76	0.63	0.64
5	assign (segid 3A4 and resid 110 and name CA) (segid 3A4 and resid 410 and name CA)	12.23	0.61	0.61
	assign (segid 3A4 and resid 110 and name CA) (segid 3A4 and resid 411 and name CA)	8.64	0.66	0.66
	assign (segid 3A4 and resid 110 and name CA) (segid 3A4 and resid 411 and name CB)	7.64	0.62	0.62
	assign (segid 3A4 and resid 110 and name CA) (segid 3A4 and resid 412 and name CA)	8.86	1.12	1.12
	assign (segid 3A4 and resid 110 and name CA) (segid 3A4 and resid 413 and name CA)	12.39	1.45	1.44
10	assign (segid 3A4 and resid 110 and name CA) (segid 3A4 and resid 414 and name CA)	12.63	1.02	1.01
	assign (segid 3A4 and resid 110 and name CA) (segid 3A4 and resid 415 and name CA)	14.99	1.12	1.12
	assign (segid 3A4 and resid 110 and name CA) (segid 3A4 and resid 415 and name CB)	15.59	1.36	1.36
	assign (segid 3A4 and resid 110 and name CA) (segid 3A4 and resid 416 and name CA)	16.59	1.15	1.14
	assign (segid 3A4 and resid 110 and name CA) (segid 3A4 and resid 417 and name CA)	17.66	1.06	1.06
15	assign (segid 3A4 and resid 110 and name CA) (segid 3A4 and resid 438 and name CA)	17.11	1.15	1.16
	assign (segid 3A4 and resid 110 and name CA) (segid 3A4 and resid 439 and name CA)	15.10	0.94	0.93
	assign (segid 3A4 and resid 110 and name CA) (segid 3A4 and resid 440 and name CA)	12.79	1.19	1.18
	assign (segid 3A4 and resid 110 and name CB) (segid 3A4 and resid 111 and name C)	5.56	0.07	0.07
	assign (segid 3A4 and resid 110 and name CB) (segid 3A4 and resid 111 and name CA)	4.49	0.06	0.06
20	assign (segid 3A4 and resid 110 and name CB) (segid 3A4 and resid 111 and name CB)	5.22	0.14	0.15
	assign (segid 3A4 and resid 110 and name CB) (segid 3A4 and resid 111 and name N)	3.19	0.07	0.07
	assign (segid 3A4 and resid 110 and name CB) (segid 3A4 and resid 111 and name O)	6.66	0.06	0.06
	assign (segid 3A4 and resid 110 and name CB) (segid 3A4 and resid 112 and name CA)	7.17	0.29	0.28
	assign (segid 3A4 and resid 110 and name CB) (segid 3A4 and resid 112 and name CB)	6.83	0.20	0.21
25	assign (segid 3A4 and resid 110 and name CB) (segid 3A4 and resid 112 and name N)	5.56	0.16	0.16
	assign (segid 3A4 and resid 110 and name CB) (segid 3A4 and resid 119 and name CA)	11.96	1.03	1.04
	assign (segid 3A4 and resid 110 and name CB) (segid 3A4 and resid 119 and name CB)	10.74	0.94	0.94
	assign (segid 3A4 and resid 110 and name CB) (segid 3A4 and resid 120 and name CA)	14.41	0.78	0.77
	assign (segid 3A4 and resid 110 and name CB) (segid 3A4 and resid 120 and name CB)	15.39	0.64	0.64
30	assign (segid 3A4 and resid 110 and name CB) (segid 3A4 and resid 121 and name CA)	13.28	1.01	1.01
	assign (segid 3A4 and resid 110 and name CB) (segid 3A4 and resid 121 and name CB)	13.53	1.07	1.08
	assign (segid 3A4 and resid 110 and name CB) (segid 3A4 and resid 122 and name CA)	16.21	1.01	1.02
	assign (segid 3A4 and resid 110 and name CB) (segid 3A4 and resid 122 and name CB)	17.62	1.01	1.00
	assign (segid 3A4 and resid 110 and name CB) (segid 3A4 and resid 123 and name CA)	15.66	0.77	0.76
35	assign (segid 3A4 and resid 110 and name CB) (segid 3A4 and resid 123 and name CB)	16.01	0.73	0.73
	assign (segid 3A4 and resid 110 and name CB) (segid 3A4 and resid 124 and name CA)	12.15	0.84	0.84
	assign (segid 3A4 and resid 110 and name CB) (segid 3A4 and resid 124 and name CB)	11.10	0.70	0.70
	assign (segid 3A4 and resid 110 and name CB) (segid 3A4 and resid 125 and name CA)	12.58	1.54	1.54
	assign (segid 3A4 and resid 110 and name CB) (segid 3A4 and resid 125 and name CB)	12.23	2.09	2.08
40	assign (segid 3A4 and resid 110 and name CB) (segid 3A4 and resid 126 and name CA)	15.72	1.44	1.45
	assign (segid 3A4 and resid 110 and name CB) (segid 3A4 and resid 127 and name CA)	16.40	0.60	0.61
	assign (segid 3A4 and resid 110 and name CB) (segid 3A4 and resid 127 and name CB)	16.29	1.06	1.05
	assign (segid 3A4 and resid 110 and name CB) (segid 3A4 and resid 128 and name CA)	15.06	0.72	0.73
	assign (segid 3A4 and resid 110 and name CB) (segid 3A4 and resid 128 and name CB)	14.02	0.79	0.78
45	assign (segid 3A4 and resid 110 and name CB) (segid 3A4 and resid 129 and name CA)	15.89	1.75	1.74
	assign (segid 3A4 and resid 110 and name CB) (segid 3A4 and resid 129 and name CB)	15.67	2.21	2.20
	assign (segid 3A4 and resid 110 and name CB) (segid 3A4 and resid 132 and name CA)	18.50	1.28	1.27
	assign (segid 3A4 and resid 110 and name CB) (segid 3A4 and resid 132 and name CB)	17.49	1.57	1.56
	assign (segid 3A4 and resid 110 and name CB) (segid 3A4 and resid 263 and name CA)	17.89	0.57	0.56
50	assign (segid 3A4 and resid 110 and name CB) (segid 3A4 and resid 263 and name CB)	16.90	0.53	0.52
	assign (segid 3A4 and resid 110 and name CB) (segid 3A4 and resid 264 and name CA)	18.10	0.70	0.70
	assign (segid 3A4 and resid 110 and name CB) (segid 3A4 and resid 267 and name CA)	16.91	1.06	1.05
	assign (segid 3A4 and resid 110 and name CB) (segid 3A4 and resid 267 and name CB)	15.74	1.02	1.02
	assign (segid 3A4 and resid 110 and name CB) (segid 3A4 and resid 400 and name CA)	18.86	0.55	0.55
55	assign (segid 3A4 and resid 110 and name CB) (segid 3A4 and resid 401 and name CA)	18.80	0.56	0.56
	assign (segid 3A4 and resid 110 and name CB) (segid 3A4 and resid 402 and name CA)	18.93	0.59	0.58
	assign (segid 3A4 and resid 110 and name CB) (segid 3A4 and resid 403 and name CA)	16.27	0.57	0.58
	assign (segid 3A4 and resid 110 and name CB) (segid 3A4 and resid 403 and name CB)	16.47	0.66	0.66
	assign (segid 3A4 and resid 110 and name CB) (segid 3A4 and resid 404 and name CA)	13.84	0.48	0.49
60	assign (segid 3A4 and resid 110 and name CB) (segid 3A4 and resid 404 and name CB)	14.25	0.49	0.49
	assign (segid 3A4 and resid 110 and name CB) (segid 3A4 and resid 405 and name CA)	14.88	0.83	0.82
	assign (segid 3A4 and resid 110 and name CB) (segid 3A4 and resid 405 and name CB)	16.27	0.86	0.86
	assign (segid 3A4 and resid 110 and name CB) (segid 3A4 and resid 406 and name CA)	15.02	0.75	0.74
	assign (segid 3A4 and resid 110 and name CB) (segid 3A4 and resid 407 and name CA)	11.54	0.62	0.63
65	assign (segid 3A4 and resid 110 and name CB) (segid 3A4 and resid 407 and name CB)	11.21	0.57	0.58
	assign (segid 3A4 and resid 110 and name CB) (segid 3A4 and resid 408 and name CA)	10.07	0.92	0.93
	assign (segid 3A4 and resid 110 and name CB) (segid 3A4 and resid 408 and name CB)	10.69	1.06	1.06
	assign (segid 3A4 and resid 110 and name CB) (segid 3A4 and resid 409 and name CA)	12.24	1.13	1.13
	assign (segid 3A4 and resid 110 and name CB) (segid 3A4 and resid 409 and name CB)	13.71	1.10	1.10
70	assign (segid 3A4 and resid 110 and name CB) (segid 3A4 and resid 410 and name CA)	11.77	1.07	1.08
	assign (segid 3A4 and resid 110 and name CB) (segid 3A4 and resid 411 and name CA)	8.19	1.20	1.19
	assign (segid 3A4 and resid 110 and name CB) (segid 3A4 and resid 411 and name CB)	7.14	1.13	1.12
	assign (segid 3A4 and resid 110 and name CB) (segid 3A4 and resid 412 and name CA)	8.96	1.56	1.57
	assign (segid 3A4 and resid 110 and name CB) (segid 3A4 and resid 413 and name CA)	12.90	1.71	1.71
75	assign (segid 3A4 and resid 110 and name CB) (segid 3A4 and resid 414 and name CA)	13.42	1.34	1.33
	assign (segid 3A4 and resid 110 and name CB) (segid 3A4 and resid 415 and name CA)	15.97	1.34	1.35
	assign (segid 3A4 and resid 110 and name CB) (segid 3A4 and resid 439 and name CA)	16.41	1.01	1.00
	assign (segid 3A4 and resid 110 and name CB) (segid 3A4 and resid 440 and name CA)	14.03	1.32	1.32
	assign (segid 3A4 and resid 110 and name N) (segid 3A4 and resid 110 and name C)	2.47	0.03	0.04
80	assign (segid 3A4 and resid 110 and name N) (segid 3A4 and resid 110 and name CA)	1.46	0.00	0.00
	assign (segid 3A4 and resid 110 and name N) (segid 3A4 and resid 110 and name CB)	2.46	0.01	0.01
	assign (segid 3A4 and resid 110 and name N) (segid 3A4 and resid 110 and name O)	3.52	0.04	0.05

	assign (segid 3A4 and resid 110 and name N)	(segid 3A4 and resid 111 and name C)	4.83	0.08	0.08
	assign (segid 3A4 and resid 110 and name N)	(segid 3A4 and resid 111 and name CA)	4.22	0.10	0.09
	assign (segid 3A4 and resid 110 and name N)	(segid 3A4 and resid 111 and name CB)	4.94	0.08	0.09
	assign (segid 3A4 and resid 110 and name N)	(segid 3A4 and resid 111 and name N)	2.80	0.09	0.09
	assign (segid 3A4 and resid 110 and name N)	(segid 3A4 and resid 111 and name O)	6.00	0.14	0.14
5	assign (segid 3A4 and resid 110 and name N)	(segid 3A4 and resid 112 and name C)	6.14	0.18	0.18
	assign (segid 3A4 and resid 110 and name N)	(segid 3A4 and resid 112 and name CA)	5.51	0.16	0.17
	assign (segid 3A4 and resid 110 and name N)	(segid 3A4 and resid 112 and name N)	4.42	0.14	0.14
	assign (segid 3A4 and resid 110 and name N)	(segid 3A4 and resid 112 and name O)	6.78	0.60	0.60
	assign (segid 3A4 and resid 110 and name N)	(segid 3A4 and resid 112 and name CB)	3.21	0.09	0.09
10	assign (segid 3A4 and resid 110 and name O)	(segid 3A4 and resid 111 and name C)	3.25	0.16	0.16
	assign (segid 3A4 and resid 110 and name O)	(segid 3A4 and resid 111 and name CA)	2.78	0.04	0.04
	assign (segid 3A4 and resid 110 and name O)	(segid 3A4 and resid 111 and name CB)	4.20	0.05	0.04
	assign (segid 3A4 and resid 110 and name O)	(segid 3A4 and resid 111 and name N)	2.24	0.01	0.02
	assign (segid 3A4 and resid 110 and name O)	(segid 3A4 and resid 111 and name O)	4.22	0.24	0.23
15	assign (segid 3A4 and resid 110 and name O)	(segid 3A4 and resid 112 and name C)	4.35	0.30	0.30
	assign (segid 3A4 and resid 110 and name O)	(segid 3A4 and resid 112 and name CA)	4.36	0.29	0.30
	assign (segid 3A4 and resid 110 and name O)	(segid 3A4 and resid 112 and name N)	3.24	0.26	0.26
	assign (segid 3A4 and resid 110 and name O)	(segid 3A4 and resid 112 and name O)	4.87	0.72	0.72
	assign (segid 3A4 and resid 110 and name O)	(segid 3A4 and resid 112 and name CB)	2.52	0.03	0.02
20	assign (segid 3A4 and resid 111 and name C)	(segid 3A4 and resid 111 and name CB)	1.24	0.01	0.01
	assign (segid 3A4 and resid 111 and name C)	(segid 3A4 and resid 112 and name C)	3.22	0.19	0.19
	assign (segid 3A4 and resid 111 and name C)	(segid 3A4 and resid 112 and name CA)	2.44	0.02	0.02
	assign (segid 3A4 and resid 111 and name C)	(segid 3A4 and resid 112 and name N)	1.33	0.00	0.00
	assign (segid 3A4 and resid 111 and name C)	(segid 3A4 and resid 112 and name O)	3.98	0.45	0.46
25	assign (segid 3A4 and resid 111 and name C)	(segid 3A4 and resid 112 and name O)	1.51	0.01	0.02
	assign (segid 3A4 and resid 111 and name CA)	(segid 3A4 and resid 111 and name CB)	1.53	0.01	0.01
	assign (segid 3A4 and resid 111 and name CA)	(segid 3A4 and resid 111 and name O)	2.40	0.02	0.01
	assign (segid 3A4 and resid 111 and name CA)	(segid 3A4 and resid 112 and name C)	4.51	0.12	0.12
	assign (segid 3A4 and resid 111 and name CA)	(segid 3A4 and resid 112 and name CA)	3.80	0.01	0.02
30	assign (segid 3A4 and resid 111 and name CA)	(segid 3A4 and resid 112 and name N)	2.44	0.02	0.02
	assign (segid 3A4 and resid 111 and name CA)	(segid 3A4 and resid 112 and name O)	5.22	0.57	0.57
	assign (segid 3A4 and resid 111 and name CA)	(segid 3A4 and resid 119 and name CA)	10.71	0.41	0.41
	assign (segid 3A4 and resid 111 and name CA)	(segid 3A4 and resid 119 and name CB)	9.70	0.61	0.61
35	assign (segid 3A4 and resid 111 and name CA)	(segid 3A4 and resid 120 and name CA)	13.39	0.64	0.64
	assign (segid 3A4 and resid 111 and name CA)	(segid 3A4 and resid 120 and name CB)	14.10	0.68	0.69
	assign (segid 3A4 and resid 111 and name CA)	(segid 3A4 and resid 121 and name CA)	13.30	1.12	1.12
	assign (segid 3A4 and resid 111 and name CA)	(segid 3A4 and resid 121 and name CB)	13.94	1.12	1.11
	assign (segid 3A4 and resid 111 and name CA)	(segid 3A4 and resid 122 and name CA)	16.03	1.40	1.40
40	assign (segid 3A4 and resid 111 and name CA)	(segid 3A4 and resid 122 and name CB)	17.31	1.39	1.38
	assign (segid 3A4 and resid 111 and name CA)	(segid 3A4 and resid 123 and name CA)	14.70	1.47	1.48
	assign (segid 3A4 and resid 111 and name CA)	(segid 3A4 and resid 123 and name CB)	14.71	1.52	1.53
	assign (segid 3A4 and resid 111 and name CA)	(segid 3A4 and resid 124 and name CA)	11.42	1.58	1.58
	assign (segid 3A4 and resid 111 and name CA)	(segid 3A4 and resid 124 and name CB)	10.29	1.40	1.41
	assign (segid 3A4 and resid 111 and name CA)	(segid 3A4 and resid 125 and name CA)	13.03	1.93	1.93
45	assign (segid 3A4 and resid 111 and name CA)	(segid 3A4 and resid 125 and name CB)	12.95	2.23	2.22
	assign (segid 3A4 and resid 111 and name CA)	(segid 3A4 and resid 126 and name CA)	16.27	1.58	1.59
	assign (segid 3A4 and resid 111 and name CA)	(segid 3A4 and resid 127 and name CA)	16.42	1.54	1.54
	assign (segid 3A4 and resid 111 and name CA)	(segid 3A4 and resid 128 and name CA)	15.43	1.60	1.60
	assign (segid 3A4 and resid 111 and name CA)	(segid 3A4 and resid 128 and name CB)	14.35	1.69	1.69
50	assign (segid 3A4 and resid 111 and name CA)	(segid 3A4 and resid 267 and name CB)	17.38	0.72	0.72
	assign (segid 3A4 and resid 111 and name CA)	(segid 3A4 and resid 404 and name CA)	16.78	0.87	0.86
	assign (segid 3A4 and resid 111 and name CA)	(segid 3A4 and resid 404 and name CB)	16.90	0.92	0.91
	assign (segid 3A4 and resid 111 and name CA)	(segid 3A4 and resid 405 and name CA)	17.96	0.90	0.91
	assign (segid 3A4 and resid 111 and name CA)	(segid 3A4 and resid 407 and name CA)	15.24	0.78	0.79
55	assign (segid 3A4 and resid 111 and name CA)	(segid 3A4 and resid 407 and name CB)	14.81	0.87	0.88
	assign (segid 3A4 and resid 111 and name CA)	(segid 3A4 and resid 408 and name CA)	13.38	0.65	0.66
	assign (segid 3A4 and resid 111 and name CA)	(segid 3A4 and resid 408 and name CB)	13.69	0.76	0.76
	assign (segid 3A4 and resid 111 and name CA)	(segid 3A4 and resid 409 and name CA)	15.67	0.54	0.55
	assign (segid 3A4 and resid 111 and name CA)	(segid 3A4 and resid 409 and name CB)	17.10	0.52	0.53
60	assign (segid 3A4 and resid 111 and name CA)	(segid 3A4 and resid 410 and name CA)	15.64	0.69	0.70
	assign (segid 3A4 and resid 111 and name CA)	(segid 3A4 and resid 411 and name CA)	12.02	0.75	0.75
	assign (segid 3A4 and resid 111 and name CA)	(segid 3A4 and resid 411 and name CB)	11.03	0.68	0.68
	assign (segid 3A4 and resid 111 and name CA)	(segid 3A4 and resid 412 and name CA)	12.07	0.92	0.92
	assign (segid 3A4 and resid 111 and name CA)	(segid 3A4 and resid 413 and name CA)	15.09	1.21	1.22
65	assign (segid 3A4 and resid 111 and name CA)	(segid 3A4 and resid 414 and name CA)	15.02	0.27	0.27
	assign (segid 3A4 and resid 111 and name CA)	(segid 3A4 and resid 415 and name CA)	16.93	0.53	0.53
	assign (segid 3A4 and resid 111 and name CA)	(segid 3A4 and resid 415 and name CB)	17.47	0.92	0.93
	assign (segid 3A4 and resid 111 and name CA)	(segid 3A4 and resid 416 and name CA)	17.99	0.78	0.78
	assign (segid 3A4 and resid 111 and name CA)	(segid 3A4 and resid 417 and name CA)	18.47	0.33	0.32
70	assign (segid 3A4 and resid 111 and name CA)	(segid 3A4 and resid 438 and name CA)	18.09	0.78	0.77
	assign (segid 3A4 and resid 111 and name CA)	(segid 3A4 and resid 439 and name CA)	15.77	0.36	0.37
	assign (segid 3A4 and resid 111 and name CA)	(segid 3A4 and resid 440 and name CA)	14.03	0.55	0.55
	assign (segid 3A4 and resid 111 and name CB)	(segid 3A4 and resid 112 and name C)	5.71	0.17	0.17
75	assign (segid 3A4 and resid 111 and name CB)	(segid 3A4 and resid 112 and name CA)	4.78	0.08	0.09
	assign (segid 3A4 and resid 111 and name CB)	(segid 3A4 and resid 112 and name N)	3.52	0.08	0.09
	assign (segid 3A4 and resid 111 and name CB)	(segid 3A4 and resid 112 and name O)	6.43	0.50	0.50
	assign (segid 3A4 and resid 111 and name CB)	(segid 3A4 and resid 119 and name CA)	11.42	0.49	0.48
	assign (segid 3A4 and resid 111 and name CB)	(segid 3A4 and resid 119 and name CB)	10.39	0.72	0.73
	assign (segid 3A4 and resid 111 and name CB)	(segid 3A4 and resid 120 and name CA)	13.84	0.89	0.89
80	assign (segid 3A4 and resid 111 and name CB)	(segid 3A4 and resid 120 and name CB)	14.44	0.98	0.99
	assign (segid 3A4 and resid 111 and name CB)	(segid 3A4 and resid 121 and name CA)	13.73	1.33	1.32
	assign (segid 3A4 and resid 111 and name CB)	(segid 3A4 and resid 121 and name CB)	14.46	1.28	1.29

	assign (segid 3A4 and resid 111 and name CB)	(segid 3A4 and resid 122 and name CA)	16.19	1.67	1.67
	assign (segid 3A4 and resid 111 and name CB)	(segid 3A4 and resid 123 and name CA)	14.60	1.80	1.81
	assign (segid 3A4 and resid 111 and name CB)	(segid 3A4 and resid 123 and name CB)	14.62	1.88	1.87
	assign (segid 3A4 and resid 111 and name CB)	(segid 3A4 and resid 124 and name CA)	11.30	1.81	1.82
5	assign (segid 3A4 and resid 111 and name CB)	(segid 3A4 and resid 124 and name CB)	10.31	1.61	1.62
	assign (segid 3A4 and resid 111 and name CB)	(segid 3A4 and resid 125 and name CA)	12.98	2.07	2.07
	assign (segid 3A4 and resid 111 and name CB)	(segid 3A4 and resid 125 and name CB)	13.04	2.27	2.28
	assign (segid 3A4 and resid 111 and name CB)	(segid 3A4 and resid 126 and name CA)	16.17	1.77	1.76
	assign (segid 3A4 and resid 111 and name CB)	(segid 3A4 and resid 128 and name CA)	14.94	1.94	1.93
	assign (segid 3A4 and resid 111 and name CB)	(segid 3A4 and resid 128 and name CB)	13.88	2.01	2.00
10	assign (segid 3A4 and resid 111 and name CB)	(segid 3A4 and resid 129 and name CA)	16.56	2.17	2.18
	assign (segid 3A4 and resid 111 and name CB)	(segid 3A4 and resid 267 and name CB)	18.05	0.83	0.83
	assign (segid 3A4 and resid 111 and name CB)	(segid 3A4 and resid 404 and name CA)	16.94	0.95	0.96
	assign (segid 3A4 and resid 111 and name CB)	(segid 3A4 and resid 404 and name CB)	17.03	1.06	1.07
	assign (segid 3A4 and resid 111 and name CB)	(segid 3A4 and resid 407 and name CA)	15.62	0.72	0.71
15	assign (segid 3A4 and resid 111 and name CB)	(segid 3A4 and resid 407 and name CB)	15.07	0.82	0.81
	assign (segid 3A4 and resid 111 and name CB)	(segid 3A4 and resid 408 and name CA)	13.97	0.61	0.62
	assign (segid 3A4 and resid 111 and name CB)	(segid 3A4 and resid 408 and name CB)	14.28	0.76	0.75
	assign (segid 3A4 and resid 111 and name CB)	(segid 3A4 and resid 409 and name CA)	16.47	0.49	0.50
	assign (segid 3A4 and resid 111 and name CB)	(segid 3A4 and resid 409 and name CB)	17.90	0.48	0.47
20	assign (segid 3A4 and resid 111 and name CB)	(segid 3A4 and resid 410 and name CA)	16.38	0.72	0.72
	assign (segid 3A4 and resid 111 and name CB)	(segid 3A4 and resid 411 and name CA)	12.83	0.83	0.82
	assign (segid 3A4 and resid 111 and name CB)	(segid 3A4 and resid 411 and name CB)	11.74	0.72	0.73
	assign (segid 3A4 and resid 111 and name CB)	(segid 3A4 and resid 412 and name CA)	13.15	0.94	0.94
	assign (segid 3A4 and resid 111 and name CB)	(segid 3A4 and resid 413 and name CA)	16.38	1.15	1.14
25	assign (segid 3A4 and resid 111 and name CB)	(segid 3A4 and resid 414 and name CA)	16.22	0.26	0.26
	assign (segid 3A4 and resid 111 and name CB)	(segid 3A4 and resid 415 and name CA)	18.13	0.43	0.43
	assign (segid 3A4 and resid 111 and name CB)	(segid 3A4 and resid 415 and name CB)	18.73	0.88	0.87
	assign (segid 3A4 and resid 111 and name CB)	(segid 3A4 and resid 439 and name CA)	16.54	0.49	0.49
	assign (segid 3A4 and resid 111 and name CB)	(segid 3A4 and resid 440 and name CA)	15.01	0.45	0.45
30	assign (segid 3A4 and resid 111 and name CB)	(segid 3A4 and resid 111 and name C)	2.50	0.03	0.04
	assign (segid 3A4 and resid 111 and name N)	(segid 3A4 and resid 111 and name CA)	1.46	0.01	0.01
	assign (segid 3A4 and resid 111 and name N)	(segid 3A4 and resid 111 and name CB)	2.42	0.02	0.03
	assign (segid 3A4 and resid 111 and name N)	(segid 3A4 and resid 111 and name O)	3.62	0.04	0.04
	assign (segid 3A4 and resid 111 and name N)	(segid 3A4 and resid 112 and name C)	4.91	0.08	0.07
35	assign (segid 3A4 and resid 111 and name N)	(segid 3A4 and resid 112 and name CA)	4.22	0.07	0.07
	assign (segid 3A4 and resid 111 and name N)	(segid 3A4 and resid 112 and name N)	2.79	0.07	0.07
	assign (segid 3A4 and resid 111 and name N)	(segid 3A4 and resid 112 and name O)	5.61	0.62	0.63
	assign (segid 3A4 and resid 111 and name O)	(segid 3A4 and resid 111 and name CB)	2.98	0.12	0.12
40	assign (segid 3A4 and resid 111 and name O)	(segid 3A4 and resid 112 and name C)	3.37	0.35	0.35
	assign (segid 3A4 and resid 111 and name O)	(segid 3A4 and resid 112 and name N)	2.75	0.05	0.05
	assign (segid 3A4 and resid 111 and name O)	(segid 3A4 and resid 112 and name O)	2.23	0.01	0.02
	assign (segid 3A4 and resid 111 and name O)	(segid 3A4 and resid 112 and name O)	4.05	0.48	0.48
	assign (segid 3A4 and resid 112 and name C)	(segid 3A4 and resid 112 and name O)	1.23	0.01	0.01
45	assign (segid 3A4 and resid 112 and name C)	(segid 3A4 and resid 112 and name C)	1.53	0.01	0.00
	assign (segid 3A4 and resid 112 and name CA)	(segid 3A4 and resid 112 and name O)	2.40	0.02	0.02
	assign (segid 3A4 and resid 112 and name CA)	(segid 3A4 and resid 119 and name CA)	7.61	0.57	0.57
	assign (segid 3A4 and resid 112 and name CA)	(segid 3A4 and resid 119 and name CB)	6.83	0.91	0.91
	assign (segid 3A4 and resid 112 and name CA)	(segid 3A4 and resid 120 and name CA)	10.64	0.80	0.79
50	assign (segid 3A4 and resid 112 and name CA)	(segid 3A4 and resid 120 and name CB)	11.38	0.72	0.72
	assign (segid 3A4 and resid 112 and name CA)	(segid 3A4 and resid 121 and name CA)	11.25	1.37	1.36
	assign (segid 3A4 and resid 112 and name CA)	(segid 3A4 and resid 121 and name CB)	11.91	1.42	1.42
	assign (segid 3A4 and resid 112 and name CA)	(segid 3A4 and resid 122 and name CA)	14.22	1.46	1.45
	assign (segid 3A4 and resid 112 and name CA)	(segid 3A4 and resid 122 and name CB)	15.33	1.43	1.43
55	assign (segid 3A4 and resid 112 and name CA)	(segid 3A4 and resid 123 and name CA)	13.06	1.34	1.33
	assign (segid 3A4 and resid 112 and name CA)	(segid 3A4 and resid 123 and name CB)	12.87	1.32	1.31
	assign (segid 3A4 and resid 112 and name CA)	(segid 3A4 and resid 124 and name CA)	10.24	1.59	1.58
	assign (segid 3A4 and resid 112 and name CA)	(segid 3A4 and resid 124 and name CB)	8.89	1.55	1.55
	assign (segid 3A4 and resid 112 and name CA)	(segid 3A4 and resid 125 and name CA)	12.34	1.91	1.92
60	assign (segid 3A4 and resid 112 and name CA)	(segid 3A4 and resid 125 and name CB)	12.14	2.23	2.23
	assign (segid 3A4 and resid 112 and name CA)	(segid 3A4 and resid 126 and name CA)	15.53	1.62	1.62
	assign (segid 3A4 and resid 112 and name CA)	(segid 3A4 and resid 127 and name CA)	15.92	1.30	1.30
	assign (segid 3A4 and resid 112 and name CA)	(segid 3A4 and resid 127 and name CB)	15.36	1.44	1.44
	assign (segid 3A4 and resid 112 and name CA)	(segid 3A4 and resid 128 and name CA)	15.58	1.35	1.35
	assign (segid 3A4 and resid 112 and name CA)	(segid 3A4 and resid 128 and name CB)	14.53	1.46	1.45
65	assign (segid 3A4 and resid 112 and name CA)	(segid 3A4 and resid 263 and name CB)	17.85	1.31	1.31
	assign (segid 3A4 and resid 112 and name CA)	(segid 3A4 and resid 264 and name CA)	17.65	1.23	1.23
	assign (segid 3A4 and resid 112 and name CA)	(segid 3A4 and resid 267 and name CA)	17.19	1.21	1.22
	assign (segid 3A4 and resid 112 and name CA)	(segid 3A4 and resid 267 and name CB)	15.84	1.21	1.22
70	assign (segid 3A4 and resid 112 and name CA)	(segid 3A4 and resid 404 and name CA)	17.37	1.32	1.32
	assign (segid 3A4 and resid 112 and name CA)	(segid 3A4 and resid 404 and name CB)	17.28	1.31	1.32
	assign (segid 3A4 and resid 112 and name CA)	(segid 3A4 and resid 407 and name CA)	16.30	1.36	1.36
	assign (segid 3A4 and resid 112 and name CA)	(segid 3A4 and resid 407 and name CB)	16.05	1.41	1.41
	assign (segid 3A4 and resid 112 and name CA)	(segid 3A4 and resid 408 and name CA)	13.71	1.29	1.29
75	assign (segid 3A4 and resid 112 and name CA)	(segid 3A4 and resid 408 and name CB)	13.71	1.34	1.33
	assign (segid 3A4 and resid 112 and name CA)	(segid 3A4 and resid 409 and name CA)	15.77	0.99	0.98
	assign (segid 3A4 and resid 112 and name CA)	(segid 3A4 and resid 409 and name CB)	17.10	0.98	0.98
	assign (segid 3A4 and resid 112 and name CA)	(segid 3A4 and resid 410 and name CA)	16.46	0.86	0.85
	assign (segid 3A4 and resid 112 and name CA)	(segid 3A4 and resid 411 and name CA)	12.95	0.77	0.76
80	assign (segid 3A4 and resid 112 and name CA)	(segid 3A4 and resid 411 and name CB)	12.12	0.88	0.87
	assign (segid 3A4 and resid 112 and name CA)	(segid 3A4 and resid 412 and name CA)	11.95	0.69	0.69
	assign (segid 3A4 and resid 112 and name CA)	(segid 3A4 and resid 413 and name CA)	13.89	1.00	1.00
	assign (segid 3A4 and resid 112 and name CA)	(segid 3A4 and resid 414 and name CA)	13.21	0.54	0.54

	assign (segid 3A4 and resid 112 and name CA)	(segid 3A4 and resid 415 and name CA)	14.48	0.73	0.73
	assign (segid 3A4 and resid 112 and name CA)	(segid 3A4 and resid 415 and name CB)	14.97	1.11	1.11
	assign (segid 3A4 and resid 112 and name CA)	(segid 3A4 and resid 416 and name CA)	15.12	0.90	0.90
	assign (segid 3A4 and resid 112 and name CA)	(segid 3A4 and resid 417 and name CA)	15.28	0.52	0.53
5	assign (segid 3A4 and resid 112 and name CA)	(segid 3A4 and resid 437 and name CA)	17.11	0.92	0.92
	assign (segid 3A4 and resid 112 and name CA)	(segid 3A4 and resid 438 and name CA)	15.36	0.85	0.84
	assign (segid 3A4 and resid 112 and name CA)	(segid 3A4 and resid 439 and name CA)	12.69	0.60	0.59
	assign (segid 3A4 and resid 112 and name CA)	(segid 3A4 and resid 440 and name CA)	11.16	0.66	0.66
	assign (segid 3A4 and resid 112 and name CA)	(segid 3A4 and resid 112 and name C)	2.43	0.03	0.03
	assign (segid 3A4 and resid 112 and name N)	(segid 3A4 and resid 112 and name CA)	1.45	0.01	0.01
10	assign (segid 3A4 and resid 112 and name N)	(segid 3A4 and resid 112 and name O)	3.28	0.35	0.35
	assign (segid 3A4 and resid 119 and name C)	(segid 3A4 and resid 119 and name CB)	2.51	0.02	0.01
	assign (segid 3A4 and resid 119 and name C)	(segid 3A4 and resid 119 and name O)	1.24	0.01	0.01
	assign (segid 3A4 and resid 119 and name C)	(segid 3A4 and resid 120 and name C)	3.19	0.10	0.10
	assign (segid 3A4 and resid 119 and name C)	(segid 3A4 and resid 120 and name CA)	2.44	0.02	0.03
15	assign (segid 3A4 and resid 119 and name C)	(segid 3A4 and resid 120 and name CB)	3.61	0.03	0.04
	assign (segid 3A4 and resid 119 and name C)	(segid 3A4 and resid 120 and name N)	1.32	0.01	0.01
	assign (segid 3A4 and resid 119 and name C)	(segid 3A4 and resid 120 and name O)	3.90	0.11	0.10
	assign (segid 3A4 and resid 119 and name C)	(segid 3A4 and resid 121 and name C)	5.96	0.11	0.12
	assign (segid 3A4 and resid 119 and name C)	(segid 3A4 and resid 121 and name CA)	4.80	0.11	0.12
20	assign (segid 3A4 and resid 119 and name C)	(segid 3A4 and resid 121 and name CB)	5.51	0.09	0.10
	assign (segid 3A4 and resid 119 and name C)	(segid 3A4 and resid 121 and name N)	3.63	0.09	0.09
	assign (segid 3A4 and resid 119 and name C)	(segid 3A4 and resid 121 and name O)	6.82	0.20	0.20
	assign (segid 3A4 and resid 119 and name C)	(segid 3A4 and resid 122 and name CA)	7.58	0.17	0.17
	assign (segid 3A4 and resid 119 and name C)	(segid 3A4 and resid 122 and name N)	6.28	0.16	0.16
25	assign (segid 3A4 and resid 119 and name C)	(segid 3A4 and resid 123 and name N)	7.20	0.26	0.26
	assign (segid 3A4 and resid 119 and name C)	(segid 3A4 and resid 123 and name C)	5.41	0.17	0.18
	assign (segid 3A4 and resid 119 and name C)	(segid 3A4 and resid 438 and name CA)	6.82	0.22	0.23
	assign (segid 3A4 and resid 119 and name C)	(segid 3A4 and resid 438 and name N)	7.06	0.34	0.35
	assign (segid 3A4 and resid 119 and name C)	(segid 3A4 and resid 438 and name O)	4.64	0.17	0.18
30	assign (segid 3A4 and resid 119 and name C)	(segid 3A4 and resid 439 and name C)	4.76	0.14	0.14
	assign (segid 3A4 and resid 119 and name C)	(segid 3A4 and resid 439 and name CA)	4.37	0.16	0.15
	assign (segid 3A4 and resid 119 and name C)	(segid 3A4 and resid 439 and name N)	5.35	0.13	0.13
	assign (segid 3A4 and resid 119 and name C)	(segid 3A4 and resid 439 and name O)	5.98	0.14	0.14
35	assign (segid 3A4 and resid 119 and name C)	(segid 3A4 and resid 440 and name C)	5.04	0.13	0.13
	assign (segid 3A4 and resid 119 and name C)	(segid 3A4 and resid 440 and name CA)	5.05	0.14	0.14
	assign (segid 3A4 and resid 119 and name C)	(segid 3A4 and resid 440 and name N)	4.08	0.14	0.15
	assign (segid 3A4 and resid 119 and name C)	(segid 3A4 and resid 440 and name O)	4.19	0.14	0.14
	assign (segid 3A4 and resid 119 and name CA)	(segid 3A4 and resid 119 and name C)	1.52	0.00	0.01
40	assign (segid 3A4 and resid 119 and name CA)	(segid 3A4 and resid 119 and name CB)	1.53	0.02	0.02
	assign (segid 3A4 and resid 119 and name CA)	(segid 3A4 and resid 119 and name O)	2.41	0.02	0.01
	assign (segid 3A4 and resid 119 and name CA)	(segid 3A4 and resid 120 and name C)	4.39	0.05	0.06
	assign (segid 3A4 and resid 119 and name CA)	(segid 3A4 and resid 120 and name CA)	3.80	0.02	0.02
	assign (segid 3A4 and resid 119 and name CA)	(segid 3A4 and resid 120 and name CB)	4.81	0.04	0.04
45	assign (segid 3A4 and resid 119 and name CA)	(segid 3A4 and resid 120 and name N)	2.43	0.03	0.03
	assign (segid 3A4 and resid 119 and name CA)	(segid 3A4 and resid 120 and name O)	4.83	0.10	0.09
	assign (segid 3A4 and resid 119 and name CA)	(segid 3A4 and resid 121 and name C)	7.02	0.16	0.16
	assign (segid 3A4 and resid 119 and name CA)	(segid 3A4 and resid 121 and name CA)	5.82	0.17	0.17
	assign (segid 3A4 and resid 119 and name CA)	(segid 3A4 and resid 121 and name CB)	6.52	0.17	0.17
50	assign (segid 3A4 and resid 119 and name CA)	(segid 3A4 and resid 121 and name N)	4.85	0.11	0.12
	assign (segid 3A4 and resid 119 and name CA)	(segid 3A4 and resid 122 and name CA)	8.76	0.17	0.17
	assign (segid 3A4 and resid 119 and name CA)	(segid 3A4 and resid 122 and name CB)	9.44	0.22	0.22
	assign (segid 3A4 and resid 119 and name CA)	(segid 3A4 and resid 122 and name N)	7.49	0.16	0.15
	assign (segid 3A4 and resid 119 and name CA)	(segid 3A4 and resid 123 and name CA)	8.65	0.39	0.38
55	assign (segid 3A4 and resid 119 and name CA)	(segid 3A4 and resid 123 and name CB)	8.36	0.33	0.32
	assign (segid 3A4 and resid 119 and name CA)	(segid 3A4 and resid 124 and name CA)	7.57	1.06	1.05
	assign (segid 3A4 and resid 119 and name CA)	(segid 3A4 and resid 124 and name CB)	6.35	1.22	1.23
	assign (segid 3A4 and resid 119 and name CA)	(segid 3A4 and resid 125 and name CA)	9.72	0.79	0.80
	assign (segid 3A4 and resid 119 and name CA)	(segid 3A4 and resid 125 and name CB)	9.34	0.86	0.86
60	assign (segid 3A4 and resid 119 and name CA)	(segid 3A4 and resid 126 and name CA)	12.08	0.86	0.85
	assign (segid 3A4 and resid 119 and name CA)	(segid 3A4 and resid 127 and name CA)	13.12	0.66	0.66
	assign (segid 3A4 and resid 119 and name CA)	(segid 3A4 and resid 127 and name CB)	12.53	0.60	0.60
	assign (segid 3A4 and resid 119 and name CA)	(segid 3A4 and resid 128 and name CA)	14.12	0.85	0.85
	assign (segid 3A4 and resid 119 and name CA)	(segid 3A4 and resid 128 and name CB)	13.34	0.95	0.96
65	assign (segid 3A4 and resid 119 and name CA)	(segid 3A4 and resid 129 and name CA)	15.88	1.10	1.11
	assign (segid 3A4 and resid 119 and name CA)	(segid 3A4 and resid 129 and name CB)	15.46	1.18	1.19
	assign (segid 3A4 and resid 119 and name CA)	(segid 3A4 and resid 130 and name CA)	18.24	0.68	0.67
	assign (segid 3A4 and resid 119 and name CA)	(segid 3A4 and resid 130 and name CB)	17.98	0.56	0.57
	assign (segid 3A4 and resid 119 and name CA)	(segid 3A4 and resid 131 and name CB)	18.15	0.77	0.78
70	assign (segid 3A4 and resid 119 and name CA)	(segid 3A4 and resid 259 and name CA)	18.94	0.47	0.47
	assign (segid 3A4 and resid 119 and name CA)	(segid 3A4 and resid 259 and name CB)	19.31	0.47	0.47
	assign (segid 3A4 and resid 119 and name CA)	(segid 3A4 and resid 260 and name CA)	15.51	0.52	0.51
	assign (segid 3A4 and resid 119 and name CA)	(segid 3A4 and resid 260 and name CB)	15.30	0.63	0.63
	assign (segid 3A4 and resid 119 and name CA)	(segid 3A4 and resid 261 and name CA)	16.19	0.54	0.53
75	assign (segid 3A4 and resid 119 and name CA)	(segid 3A4 and resid 262 and name CA)	17.55	0.51	0.51
	assign (segid 3A4 and resid 119 and name CA)	(segid 3A4 and resid 262 and name CB)	18.70	0.52	0.51
	assign (segid 3A4 and resid 119 and name CA)	(segid 3A4 and resid 263 and name CA)	14.64	0.48	0.48
	assign (segid 3A4 and resid 119 and name CA)	(segid 3A4 and resid 263 and name CB)	14.15	0.48	0.48
	assign (segid 3A4 and resid 119 and name CA)	(segid 3A4 and resid 264 and name CA)	12.37	0.45	0.46
80	assign (segid 3A4 and resid 119 and name CA)	(segid 3A4 and resid 265 and name CA)	15.35	0.52	0.52
	assign (segid 3A4 and resid 119 and name CA)	(segid 3A4 and resid 266 and name CA)	15.91	0.50	0.49
	assign (segid 3A4 and resid 119 and name CA)	(segid 3A4 and resid 267 and name CA)	12.61	0.53	0.52
	assign (segid 3A4 and resid 119 and name CA)	(segid 3A4 and resid 267 and name CB)	11.24	0.49	0.50

assign (segid 3A4 and resid 119 and name CA) (segid 3A4 and resid 268 and name CA) 13.24 0.61 0.61
 assign (segid 3A4 and resid 119 and name CA) (segid 3A4 and resid 268 and name CB) 13.60 0.56 0.56
 assign (segid 3A4 and resid 119 and name CA) (segid 3A4 and resid 269 and name CA) 16.75 0.65 0.65
 assign (segid 3A4 and resid 119 and name CA) (segid 3A4 and resid 270 and name CA) 16.14 0.79 0.78
 assign (segid 3A4 and resid 119 and name CA) (segid 3A4 and resid 270 and name CB) 15.67 0.76 0.75
 5 assign (segid 3A4 and resid 119 and name CA) (segid 3A4 and resid 271 and name CA) 13.92 0.89 0.89
 assign (segid 3A4 and resid 119 and name CA) (segid 3A4 and resid 271 and name CB) 12.61 0.90 0.90
 assign (segid 3A4 and resid 119 and name CA) (segid 3A4 and resid 272 and name CA) 16.82 0.87 0.87
 assign (segid 3A4 and resid 119 and name CA) (segid 3A4 and resid 272 and name CB) 17.20 0.85 0.84
 assign (segid 3A4 and resid 119 and name CA) (segid 3A4 and resid 277 and name CB) 17.68 0.67 0.67
 10 assign (segid 3A4 and resid 119 and name CA) (segid 3A4 and resid 404 and name CA) 16.51 0.83 0.84
 assign (segid 3A4 and resid 119 and name CA) (segid 3A4 and resid 404 and name CB) 15.93 0.80 0.80
 assign (segid 3A4 and resid 119 and name CA) (segid 3A4 and resid 405 and name CA) 16.65 0.83 0.83
 assign (segid 3A4 and resid 119 and name CA) (segid 3A4 and resid 405 and name CB) 17.41 0.77 0.77
 assign (segid 3A4 and resid 119 and name CA) (segid 3A4 and resid 407 and name CA) 17.06 0.91 0.91
 15 assign (segid 3A4 and resid 119 and name CA) (segid 3A4 and resid 407 and name CB) 17.03 0.97 0.96
 assign (segid 3A4 and resid 119 and name CA) (segid 3A4 and resid 408 and name CA) 13.65 0.83 0.84
 assign (segid 3A4 and resid 119 and name CA) (segid 3A4 and resid 408 and name CB) 12.90 0.76 0.75
 assign (segid 3A4 and resid 119 and name CA) (segid 3A4 and resid 409 and name CA) 15.44 0.59 0.58
 assign (segid 3A4 and resid 119 and name CA) (segid 3A4 and resid 409 and name CB) 16.33 0.57 0.58
 20 assign (segid 3A4 and resid 119 and name CA) (segid 3A4 and resid 410 and name CA) 17.65 0.66 0.65
 assign (segid 3A4 and resid 119 and name CA) (segid 3A4 and resid 411 and name CA) 15.08 0.64 0.65
 assign (segid 3A4 and resid 119 and name CA) (segid 3A4 and resid 411 and name CB) 14.44 0.71 0.72
 assign (segid 3A4 and resid 119 and name CA) (segid 3A4 and resid 412 and name CA) 12.85 0.62 0.62
 25 assign (segid 3A4 and resid 119 and name CA) (segid 3A4 and resid 413 and name CA) 13.05 0.96 0.96
 assign (segid 3A4 and resid 119 and name CA) (segid 3A4 and resid 414 and name CA) 10.76 0.30 0.30
 assign (segid 3A4 and resid 119 and name CA) (segid 3A4 and resid 415 and name CA) 10.58 0.31 0.30
 assign (segid 3A4 and resid 119 and name CA) (segid 3A4 and resid 415 and name CB) 11.27 0.39 0.38
 assign (segid 3A4 and resid 119 and name CA) (segid 3A4 and resid 416 and name CA) 9.88 0.27 0.28
 30 assign (segid 3A4 and resid 119 and name CA) (segid 3A4 and resid 417 and name CA) 10.08 1.19 1.19
 assign (segid 3A4 and resid 119 and name CA) (segid 3A4 and resid 423 and name CA) 14.47 1.44 1.44
 assign (segid 3A4 and resid 119 and name CA) (segid 3A4 and resid 424 and name CA) 14.74 1.21 1.20
 assign (segid 3A4 and resid 119 and name CA) (segid 3A4 and resid 425 and name CA) 15.68 1.65 1.66
 assign (segid 3A4 and resid 119 and name CA) (segid 3A4 and resid 426 and name CA) 17.47 0.99 1.00
 35 assign (segid 3A4 and resid 119 and name CA) (segid 3A4 and resid 434 and name CA) 17.52 0.78 0.77
 assign (segid 3A4 and resid 119 and name CA) (segid 3A4 and resid 435 and name CA) 14.53 0.51 0.51
 assign (segid 3A4 and resid 119 and name CA) (segid 3A4 and resid 436 and name CA) 13.40 0.37 0.38
 assign (segid 3A4 and resid 119 and name CA) (segid 3A4 and resid 437 and name CA) 10.06 0.34 0.35
 assign (segid 3A4 and resid 119 and name CA) (segid 3A4 and resid 438 and name C) 6.80 0.16 0.15
 40 assign (segid 3A4 and resid 119 and name CA) (segid 3A4 and resid 438 and name CA) 8.23 0.19 0.19
 assign (segid 3A4 and resid 119 and name CA) (segid 3A4 and resid 438 and name O) 6.05 0.18 0.18
 assign (segid 3A4 and resid 119 and name CA) (segid 3A4 and resid 439 and name C) 5.67 0.24 0.24
 assign (segid 3A4 and resid 119 and name CA) (segid 3A4 and resid 439 and name CA) 5.50 0.26 0.26
 assign (segid 3A4 and resid 119 and name CA) (segid 3A4 and resid 439 and name N) 6.63 0.18 0.17
 assign (segid 3A4 and resid 119 and name CA) (segid 3A4 and resid 439 and name O) 6.84 0.23 0.24
 45 assign (segid 3A4 and resid 119 and name CA) (segid 3A4 and resid 440 and name C) 5.07 0.25 0.24
 assign (segid 3A4 and resid 119 and name CA) (segid 3A4 and resid 440 and name CA) 5.48 0.20 0.19
 assign (segid 3A4 and resid 119 and name CA) (segid 3A4 and resid 440 and name N) 4.79 0.23 0.24
 assign (segid 3A4 and resid 119 and name CA) (segid 3A4 and resid 440 and name O) 4.04 0.27 0.27
 assign (segid 3A4 and resid 119 and name CB) (segid 3A4 and resid 120 and name C) 4.50 0.12 0.12
 50 assign (segid 3A4 and resid 119 and name CB) (segid 3A4 and resid 120 and name CA) 4.41 0.10 0.10
 assign (segid 3A4 and resid 119 and name CB) (segid 3A4 and resid 120 and name CB) 5.50 0.13 0.13
 assign (segid 3A4 and resid 119 and name CB) (segid 3A4 and resid 120 and name N) 3.13 0.13 0.12
 assign (segid 3A4 and resid 119 and name CB) (segid 3A4 and resid 120 and name O) 4.69 0.22 0.22
 55 assign (segid 3A4 and resid 119 and name CB) (segid 3A4 and resid 121 and name C) 6.67 0.26 0.26
 assign (segid 3A4 and resid 119 and name CB) (segid 3A4 and resid 121 and name CA) 5.47 0.26 0.26
 assign (segid 3A4 and resid 119 and name CB) (segid 3A4 and resid 121 and name CB) 6.18 0.31 0.30
 assign (segid 3A4 and resid 119 and name CB) (segid 3A4 and resid 121 and name N) 4.84 0.20 0.20
 assign (segid 3A4 and resid 119 and name CB) (segid 3A4 and resid 121 and name O) 7.18 0.36 0.36
 60 assign (segid 3A4 and resid 119 and name CB) (segid 3A4 and resid 122 and name CA) 8.62 0.28 0.27
 assign (segid 3A4 and resid 119 and name CB) (segid 3A4 and resid 122 and name CB) 9.49 0.22 0.23
 assign (segid 3A4 and resid 119 and name CB) (segid 3A4 and resid 122 and name N) 7.36 0.25 0.24
 assign (segid 3A4 and resid 119 and name CB) (segid 3A4 and resid 123 and name CA) 8.44 0.42 0.43
 assign (segid 3A4 and resid 119 and name CB) (segid 3A4 and resid 123 and name CB) 8.32 0.25 0.26
 65 assign (segid 3A4 and resid 119 and name CB) (segid 3A4 and resid 124 and name CA) 6.79 1.10 1.10
 assign (segid 3A4 and resid 119 and name CB) (segid 3A4 and resid 124 and name CB) 5.47 1.25 1.24
 assign (segid 3A4 and resid 119 and name CB) (segid 3A4 and resid 125 and name CA) 8.80 0.97 0.97
 assign (segid 3A4 and resid 119 and name CB) (segid 3A4 and resid 125 and name CB) 8.39 1.09 1.09
 assign (segid 3A4 and resid 119 and name CB) (segid 3A4 and resid 126 and name CA) 11.45 1.01 1.00
 70 assign (segid 3A4 and resid 119 and name CB) (segid 3A4 and resid 127 and name CA) 12.52 0.62 0.62
 assign (segid 3A4 and resid 119 and name CB) (segid 3A4 and resid 127 and name CB) 12.00 0.46 0.46
 assign (segid 3A4 and resid 119 and name CB) (segid 3A4 and resid 128 and name CA) 13.22 0.82 0.82
 assign (segid 3A4 and resid 119 and name CB) (segid 3A4 and resid 128 and name CB) 12.37 0.93 0.93
 assign (segid 3A4 and resid 119 and name CB) (segid 3A4 and resid 129 and name CA) 14.92 1.25 1.24
 75 assign (segid 3A4 and resid 119 and name CB) (segid 3A4 and resid 129 and name CB) 14.50 1.38 1.38
 assign (segid 3A4 and resid 119 and name CB) (segid 3A4 and resid 130 and name CA) 17.44 0.78 0.77
 assign (segid 3A4 and resid 119 and name CB) (segid 3A4 and resid 130 and name CB) 17.27 0.64 0.64
 assign (segid 3A4 and resid 119 and name CB) (segid 3A4 and resid 131 and name CA) 18.12 0.74 0.75
 assign (segid 3A4 and resid 119 and name CB) (segid 3A4 and resid 131 and name CB) 17.36 0.68 0.68
 80 assign (segid 3A4 and resid 119 and name CB) (segid 3A4 and resid 259 and name CA) 18.35 0.61 0.61
 assign (segid 3A4 and resid 119 and name CB) (segid 3A4 and resid 259 and name CB) 18.63 0.59 0.59
 assign (segid 3A4 and resid 119 and name CB) (segid 3A4 and resid 260 and name CA) 15.02 0.61 0.61
 assign (segid 3A4 and resid 119 and name CB) (segid 3A4 and resid 260 and name CB) 14.87 0.66 0.67

assign (segid 3A4 and resid 119 and name CB) (segid 3A4 and resid 261 and name CA) 15.97 0.66 0.66
assign (segid 3A4 and resid 119 and name CB) (segid 3A4 and resid 262 and name CA) 17.15 0.68 0.69
assign (segid 3A4 and resid 119 and name CB) (segid 3A4 and resid 262 and name CB) 18.22 0.69 0.69
assign (segid 3A4 and resid 119 and name CB) (segid 3A4 and resid 263 and name CA) 14.06 0.69 0.68
5 assign (segid 3A4 and resid 119 and name CB) (segid 3A4 and resid 263 and name CB) 13.47 0.66 0.66
assign (segid 3A4 and resid 119 and name CB) (segid 3A4 and resid 264 and name CA) 12.12 0.64 0.64
assign (segid 3A4 and resid 119 and name CB) (segid 3A4 and resid 265 and name CA) 15.24 0.72 0.71
assign (segid 3A4 and resid 119 and name CB) (segid 3A4 and resid 266 and name CA) 15.53 0.73 0.73
assign (segid 3A4 and resid 119 and name CB) (segid 3A4 and resid 267 and name CA) 12.26 0.79 0.79
10 assign (segid 3A4 and resid 119 and name CB) (segid 3A4 and resid 267 and name CB) 10.85 0.77 0.76
assign (segid 3A4 and resid 119 and name CB) (segid 3A4 and resid 268 and name CA) 13.31 0.86 0.87
assign (segid 3A4 and resid 119 and name CB) (segid 3A4 and resid 268 and name CB) 13.76 0.80 0.80
assign (segid 3A4 and resid 119 and name CB) (segid 3A4 and resid 269 and name CA) 16.71 0.91 0.90
assign (segid 3A4 and resid 119 and name CB) (segid 3A4 and resid 270 and name CA) 15.89 1.03 1.03
15 assign (segid 3A4 and resid 119 and name CB) (segid 3A4 and resid 270 and name CB) 15.30 1.00 0.99
assign (segid 3A4 and resid 119 and name CB) (segid 3A4 and resid 271 and name CA) 13.93 1.11 1.11
assign (segid 3A4 and resid 119 and name CB) (segid 3A4 and resid 271 and name CB) 12.69 1.14 1.15
assign (segid 3A4 and resid 119 and name CB) (segid 3A4 and resid 272 and name CA) 17.03 1.10 1.09
assign (segid 3A4 and resid 119 and name CB) (segid 3A4 and resid 272 and name CB) 17.45 1.08 1.08
20 assign (segid 3A4 and resid 119 and name CB) (segid 3A4 and resid 277 and name CA) 18.42 0.94 0.94
assign (segid 3A4 and resid 119 and name CB) (segid 3A4 and resid 277 and name CB) 17.25 0.91 0.92
assign (segid 3A4 and resid 119 and name CB) (segid 3A4 and resid 401 and name CA) 18.49 0.94 0.94
assign (segid 3A4 and resid 119 and name CB) (segid 3A4 and resid 404 and name CA) 15.38 0.95 0.96
assign (segid 3A4 and resid 119 and name CB) (segid 3A4 and resid 404 and name CB) 14.86 0.92 0.93
25 assign (segid 3A4 and resid 119 and name CB) (segid 3A4 and resid 405 and name CA) 15.66 1.02 1.01
assign (segid 3A4 and resid 119 and name CB) (segid 3A4 and resid 405 and name CB) 16.49 0.95 0.96
assign (segid 3A4 and resid 119 and name CB) (segid 3A4 and resid 406 and name CA) 17.93 1.03 1.04
assign (segid 3A4 and resid 119 and name CB) (segid 3A4 and resid 407 and name CA) 15.82 1.01 1.01
assign (segid 3A4 and resid 119 and name CB) (segid 3A4 and resid 407 and name CB) 15.74 1.04 1.05
30 assign (segid 3A4 and resid 119 and name CB) (segid 3A4 and resid 408 and name CA) 12.50 0.96 0.96
assign (segid 3A4 and resid 119 and name CB) (segid 3A4 and resid 408 and name CB) 11.79 0.90 0.91
assign (segid 3A4 and resid 119 and name CB) (segid 3A4 and resid 409 and name CA) 14.46 0.74 0.75
assign (segid 3A4 and resid 119 and name CB) (segid 3A4 and resid 409 and name CB) 15.42 0.74 0.74
35 assign (segid 3A4 and resid 119 and name CB) (segid 3A4 and resid 410 and name CA) 16.56 0.77 0.77
assign (segid 3A4 and resid 119 and name CB) (segid 3A4 and resid 411 and name CA) 13.94 0.68 0.67
assign (segid 3A4 and resid 119 and name CB) (segid 3A4 and resid 411 and name CB) 13.23 0.71 0.72
assign (segid 3A4 and resid 119 and name CB) (segid 3A4 and resid 412 and name CA) 11.92 0.74 0.74
assign (segid 3A4 and resid 119 and name CB) (segid 3A4 and resid 413 and name CA) 12.60 1.01 1.01
40 assign (segid 3A4 and resid 119 and name CB) (segid 3A4 and resid 414 and name CA) 10.49 0.58 0.59
assign (segid 3A4 and resid 119 and name CB) (segid 3A4 and resid 415 and name CA) 10.77 0.50 0.49
assign (segid 3A4 and resid 119 and name CB) (segid 3A4 and resid 415 and name CB) 11.51 0.66 0.65
assign (segid 3A4 and resid 119 and name CB) (segid 3A4 and resid 416 and name CA) 10.49 0.24 0.24
assign (segid 3A4 and resid 119 and name CB) (segid 3A4 and resid 417 and name CA) 11.02 1.18 1.17
45 assign (segid 3A4 and resid 119 and name CB) (segid 3A4 and resid 423 and name CA) 15.48 1.60 1.60
assign (segid 3A4 and resid 119 and name CB) (segid 3A4 and resid 424 and name CA) 15.56 1.11 1.12
assign (segid 3A4 and resid 119 and name CB) (segid 3A4 and resid 434 and name CA) 17.72 0.93 0.93
assign (segid 3A4 and resid 119 and name CB) (segid 3A4 and resid 435 and name CA) 14.87 0.68 0.68
assign (segid 3A4 and resid 119 and name CB) (segid 3A4 and resid 436 and name CA) 13.93 0.51 0.52
50 assign (segid 3A4 and resid 119 and name CB) (segid 3A4 and resid 437 and name CA) 10.78 0.45 0.46
assign (segid 3A4 and resid 119 and name CB) (segid 3A4 and resid 438 and name C) 7.51 0.23 0.24
assign (segid 3A4 and resid 119 and name CB) (segid 3A4 and resid 438 and name CA) 8.88 0.29 0.28
assign (segid 3A4 and resid 119 and name CB) (segid 3A4 and resid 438 and name O) 6.65 0.32 0.31
55 assign (segid 3A4 and resid 119 and name CB) (segid 3A4 and resid 439 and name C) 6.50 0.34 0.35
assign (segid 3A4 and resid 119 and name CB) (segid 3A4 and resid 439 and name CA) 6.50 0.30 0.30
assign (segid 3A4 and resid 119 and name CB) (segid 3A4 and resid 439 and name N) 7.52 0.20 0.19
assign (segid 3A4 and resid 119 and name CB) (segid 3A4 and resid 440 and name C) 5.48 0.51 0.51
assign (segid 3A4 and resid 119 and name CB) (segid 3A4 and resid 440 and name CA) 5.92 0.40 0.41
assign (segid 3A4 and resid 119 and name CB) (segid 3A4 and resid 440 and name N) 5.48 0.37 0.37
60 assign (segid 3A4 and resid 119 and name CB) (segid 3A4 and resid 440 and name O) 4.55 0.56 0.57
assign (segid 3A4 and resid 119 and name CB) (segid 3A4 and resid 119 and name C) 2.44 0.03 0.02
assign (segid 3A4 and resid 119 and name N) (segid 3A4 and resid 119 and name CA) 1.46 0.01 0.02
assign (segid 3A4 and resid 119 and name N) (segid 3A4 and resid 119 and name CB) 2.45 0.05 0.05
65 assign (segid 3A4 and resid 119 and name N) (segid 3A4 and resid 119 and name O) 2.70 0.05 0.04
assign (segid 3A4 and resid 119 and name N) (segid 3A4 and resid 120 and name C) 5.52 0.10 0.11
assign (segid 3A4 and resid 119 and name N) (segid 3A4 and resid 120 and name CA) 4.86 0.05 0.04
assign (segid 3A4 and resid 119 and name N) (segid 3A4 and resid 120 and name CB) 5.91 0.06 0.06
70 assign (segid 3A4 and resid 119 and name N) (segid 3A4 and resid 120 and name N) 3.62 0.03 0.02
assign (segid 3A4 and resid 119 and name N) (segid 3A4 and resid 120 and name O) 6.12 0.13 0.12
assign (segid 3A4 and resid 119 and name N) (segid 3A4 and resid 121 and name CA) 6.74 0.21 0.21
assign (segid 3A4 and resid 119 and name N) (segid 3A4 and resid 121 and name CB) 7.19 0.19 0.19
75 assign (segid 3A4 and resid 119 and name N) (segid 3A4 and resid 121 and name N) 5.78 0.16 0.16
assign (segid 3A4 and resid 119 and name N) (segid 3A4 and resid 438 and name C) 7.02 0.21 0.20
assign (segid 3A4 and resid 119 and name N) (segid 3A4 and resid 438 and name O) 6.40 0.21 0.21
80 assign (segid 3A4 and resid 119 and name N) (segid 3A4 and resid 439 and name C) 5.25 0.32 0.32
assign (segid 3A4 and resid 119 and name N) (segid 3A4 and resid 439 and name CA) 5.35 0.36 0.37
assign (segid 3A4 and resid 119 and name N) (segid 3A4 and resid 439 and name N) 6.64 0.29 0.30
assign (segid 3A4 and resid 119 and name N) (segid 3A4 and resid 439 and name O) 6.32 0.31 0.31
assign (segid 3A4 and resid 119 and name N) (segid 3A4 and resid 440 and name C) 4.08 0.18 0.18
assign (segid 3A4 and resid 119 and name N) (segid 3A4 and resid 440 and name CA) 4.75 0.21 0.21
assign (segid 3A4 and resid 119 and name N) (segid 3A4 and resid 440 and name N) 4.28 0.28 0.28
80 assign (segid 3A4 and resid 119 and name N) (segid 3A4 and resid 440 and name O) 2.98 0.16 0.16
assign (segid 3A4 and resid 119 and name O) (segid 3A4 and resid 119 and name CB) 3.32 0.08 0.08
assign (segid 3A4 and resid 119 and name O) (segid 3A4 and resid 120 and name C) 3.50 0.12 0.11

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	assign (segid 3A4 and resid 119 and name O)	(segid 3A4 and resid 120 and name CA)	2.78	0.05	0.04
	assign (segid 3A4 and resid 119 and name O)	(segid 3A4 and resid 120 and name CB)	4.07	0.06	0.06
	assign (segid 3A4 and resid 119 and name O)	(segid 3A4 and resid 120 and name N)	2.23	0.02	0.02
	assign (segid 3A4 and resid 119 and name O)	(segid 3A4 and resid 120 and name O)	4.47	0.13	0.12
	assign (segid 3A4 and resid 119 and name O)	(segid 3A4 and resid 121 and name C)	6.02	0.16	0.16
5	assign (segid 3A4 and resid 119 and name O)	(segid 3A4 and resid 121 and name CA)	4.75	0.18	0.17
	assign (segid 3A4 and resid 119 and name O)	(segid 3A4 and resid 121 and name CB)	5.14	0.14	0.15
	assign (segid 3A4 and resid 119 and name O)	(segid 3A4 and resid 121 and name N)	3.55	0.14	0.14
	assign (segid 3A4 and resid 119 and name O)	(segid 3A4 and resid 121 and name O)	6.97	0.19	0.20
	assign (segid 3A4 and resid 119 and name O)	(segid 3A4 and resid 122 and name N)	6.29	0.18	0.18
10	assign (segid 3A4 and resid 119 and name O)	(segid 3A4 and resid 437 and name C)	7.44	0.24	0.25
	assign (segid 3A4 and resid 119 and name O)	(segid 3A4 and resid 438 and name C)	4.50	0.16	0.17
	assign (segid 3A4 and resid 119 and name O)	(segid 3A4 and resid 438 and name CA)	5.98	0.19	0.19
	assign (segid 3A4 and resid 119 and name O)	(segid 3A4 and resid 438 and name N)	6.41	0.25	0.25
	assign (segid 3A4 and resid 119 and name O)	(segid 3A4 and resid 438 and name O)	3.81	0.20	0.19
15	assign (segid 3A4 and resid 119 and name O)	(segid 3A4 and resid 439 and name C)	3.56	0.12	0.13
	assign (segid 3A4 and resid 119 and name O)	(segid 3A4 and resid 439 and name CA)	3.31	0.16	0.17
	assign (segid 3A4 and resid 119 and name O)	(segid 3A4 and resid 439 and name N)	4.36	0.12	0.12
	assign (segid 3A4 and resid 119 and name O)	(segid 3A4 and resid 439 and name O)	4.78	0.13	0.13
20	assign (segid 3A4 and resid 119 and name O)	(segid 3A4 and resid 440 and name C)	4.17	0.13	0.13
	assign (segid 3A4 and resid 119 and name O)	(segid 3A4 and resid 440 and name CA)	3.96	0.17	0.18
	assign (segid 3A4 and resid 119 and name O)	(segid 3A4 and resid 440 and name N)	2.91	0.15	0.14
	assign (segid 3A4 and resid 119 and name O)	(segid 3A4 and resid 440 and name O)	3.49	0.08	0.08
	assign (segid 3A4 and resid 11 and name C)	(segid 3A4 and resid 11 and name CB)	2.51	0.01	0.02
25	assign (segid 3A4 and resid 11 and name C)	(segid 3A4 and resid 11 and name O)	1.24	0.01	0.00
	assign (segid 3A4 and resid 11 and name C)	(segid 3A4 and resid 12 and name C)	2.96	0.07	0.07
	assign (segid 3A4 and resid 11 and name C)	(segid 3A4 and resid 12 and name CA)	2.43	0.01	0.01
	assign (segid 3A4 and resid 11 and name C)	(segid 3A4 and resid 12 and name CB)	3.73	0.03	0.03
	assign (segid 3A4 and resid 11 and name C)	(segid 3A4 and resid 12 and name N)	1.33	0.01	0.01
30	assign (segid 3A4 and resid 11 and name C)	(segid 3A4 and resid 12 and name O)	3.80	0.15	0.14
	assign (segid 3A4 and resid 11 and name C)	(segid 3A4 and resid 13 and name C)	4.48	0.06	0.06
	assign (segid 3A4 and resid 11 and name C)	(segid 3A4 and resid 13 and name CA)	4.35	0.09	0.10
	assign (segid 3A4 and resid 11 and name C)	(segid 3A4 and resid 13 and name CB)	5.08	0.13	0.13
	assign (segid 3A4 and resid 11 and name C)	(segid 3A4 and resid 13 and name N)	3.19	0.10	0.11
35	assign (segid 3A4 and resid 11 and name C)	(segid 3A4 and resid 13 and name O)	5.54	0.09	0.09
	assign (segid 3A4 and resid 11 and name CA)	(segid 3A4 and resid 11 and name C)	1.53	0.00	0.01
	assign (segid 3A4 and resid 11 and name CA)	(segid 3A4 and resid 11 and name CB)	1.53	0.01	0.01
	assign (segid 3A4 and resid 11 and name CA)	(segid 3A4 and resid 11 and name O)	2.40	0.01	0.01
	assign (segid 3A4 and resid 11 and name CA)	(segid 3A4 and resid 12 and name C)	4.35	0.07	0.08
40	assign (segid 3A4 and resid 11 and name CA)	(segid 3A4 and resid 12 and name CA)	3.83	0.03	0.02
	assign (segid 3A4 and resid 11 and name CA)	(segid 3A4 and resid 12 and name CB)	4.92	0.06	0.05
	assign (segid 3A4 and resid 11 and name CA)	(segid 3A4 and resid 12 and name N)	2.46	0.03	0.03
	assign (segid 3A4 and resid 11 and name CA)	(segid 3A4 and resid 12 and name O)	5.25	0.15	0.15
	assign (segid 3A4 and resid 11 and name CA)	(segid 3A4 and resid 13 and name C)	5.34	0.10	0.10
45	assign (segid 3A4 and resid 11 and name CA)	(segid 3A4 and resid 13 and name CA)	5.29	0.13	0.12
	assign (segid 3A4 and resid 11 and name CA)	(segid 3A4 and resid 13 and name CB)	5.66	0.20	0.20
	assign (segid 3A4 and resid 11 and name CA)	(segid 3A4 and resid 13 and name N)	4.27	0.12	0.11
	assign (segid 3A4 and resid 11 and name CA)	(segid 3A4 and resid 13 and name O)	6.45	0.10	0.10
50	assign (segid 3A4 and resid 11 and name CA)	(segid 3A4 and resid 19 and name CA)	9.32	1.70	1.70
	assign (segid 3A4 and resid 11 and name CA)	(segid 3A4 and resid 19 and name CB)	10.32	1.68	1.69
	assign (segid 3A4 and resid 11 and name CA)	(segid 3A4 and resid 20 and name CA)	11.39	1.49	1.49
	assign (segid 3A4 and resid 11 and name CA)	(segid 3A4 and resid 20 and name CB)	12.77	1.46	1.45
	assign (segid 3A4 and resid 11 and name CA)	(segid 3A4 and resid 21 and name CA)	11.60	1.63	1.63
	assign (segid 3A4 and resid 11 and name CA)	(segid 3A4 and resid 21 and name CB)	10.52	1.69	1.69
55	assign (segid 3A4 and resid 11 and name CA)	(segid 3A4 and resid 22 and name CA)	13.92	1.63	1.63
	assign (segid 3A4 and resid 11 and name CA)	(segid 3A4 and resid 23 and name CA)	13.69	1.35	1.35
	assign (segid 3A4 and resid 11 and name CA)	(segid 3A4 and resid 23 and name CB)	12.73	1.27	1.26
	assign (segid 3A4 and resid 11 and name CA)	(segid 3A4 and resid 24 and name CA)	16.92	1.25	1.25
	assign (segid 3A4 and resid 11 and name CA)	(segid 3A4 and resid 25 and name CA)	17.68	0.98	0.97
60	assign (segid 3A4 and resid 11 and name CA)	(segid 3A4 and resid 30 and name CA)	16.45	1.34	1.35
	assign (segid 3A4 and resid 11 and name CA)	(segid 3A4 and resid 314 and name CA)	15.85	1.63	1.64
	assign (segid 3A4 and resid 11 and name CA)	(segid 3A4 and resid 314 and name CB)	16.20	1.60	1.60
	assign (segid 3A4 and resid 11 and name CA)	(segid 3A4 and resid 315 and name CA)	14.56	2.03	2.03
	assign (segid 3A4 and resid 11 and name CA)	(segid 3A4 and resid 315 and name CB)	15.51	2.13	2.13
65	assign (segid 3A4 and resid 11 and name CA)	(segid 3A4 and resid 316 and name CA)	15.02	2.24	2.25
	assign (segid 3A4 and resid 11 and name CA)	(segid 3A4 and resid 317 and name CA)	14.54	1.61	1.62
	assign (segid 3A4 and resid 11 and name CA)	(segid 3A4 and resid 319 and name CA)	16.28	1.88	1.88
	assign (segid 3A4 and resid 11 and name CA)	(segid 3A4 and resid 31 and name CA)	14.34	1.26	1.25
	assign (segid 3A4 and resid 11 and name CA)	(segid 3A4 and resid 31 and name CB)	15.12	1.23	1.24
70	assign (segid 3A4 and resid 11 and name CA)	(segid 3A4 and resid 32 and name CA)	11.10	1.11	1.10
	assign (segid 3A4 and resid 11 and name CA)	(segid 3A4 and resid 32 and name CB)	10.01	1.15	1.16
	assign (segid 3A4 and resid 11 and name CA)	(segid 3A4 and resid 33 and name CA)	10.92	0.92	0.92
	assign (segid 3A4 and resid 11 and name CA)	(segid 3A4 and resid 33 and name CB)	12.15	0.85	0.85
	assign (segid 3A4 and resid 11 and name CA)	(segid 3A4 and resid 343 and name CA)	16.54	1.12	1.12
75	assign (segid 3A4 and resid 11 and name CA)	(segid 3A4 and resid 343 and name CB)	16.88	1.05	1.04
	assign (segid 3A4 and resid 11 and name CA)	(segid 3A4 and resid 344 and name CA)	14.07	1.14	1.13
	assign (segid 3A4 and resid 11 and name CA)	(segid 3A4 and resid 344 and name CB)	13.44	1.13	1.12
	assign (segid 3A4 and resid 11 and name CA)	(segid 3A4 and resid 345 and name CA)	12.96	1.15	1.15
	assign (segid 3A4 and resid 11 and name CA)	(segid 3A4 and resid 345 and name CB)	14.12	1.13	1.12
80	assign (segid 3A4 and resid 11 and name CA)	(segid 3A4 and resid 346 and name CA)	10.27	1.31	1.30
	assign (segid 3A4 and resid 11 and name CA)	(segid 3A4 and resid 346 and name CB)	8.94	1.29	1.30
	assign (segid 3A4 and resid 11 and name CA)	(segid 3A4 and resid 347 and name CA)	12.11	1.12	1.13
	assign (segid 3A4 and resid 11 and name CA)	(segid 3A4 and resid 347 and name CB)	13.42	1.23	1.23

	assign (segid 3A4 and resid 11 and name CA) (segid 3A4 and resid 348 and name CA)	10.14	1.33	1.34
	assign (segid 3A4 and resid 11 and name CA) (segid 3A4 and resid 349 and name CA)	7.63	0.76	0.76
	assign (segid 3A4 and resid 11 and name CA) (segid 3A4 and resid 349 and name CB)	7.01	0.60	0.60
	assign (segid 3A4 and resid 11 and name CA) (segid 3A4 and resid 34 and name CA)	8.17	0.54	0.55
	assign (segid 3A4 and resid 11 and name CA) (segid 3A4 and resid 34 and name CB)	7.07	0.76	0.76
5	assign (segid 3A4 and resid 11 and name CA) (segid 3A4 and resid 350 and name CA)	10.48	0.62	0.61
	assign (segid 3A4 and resid 11 and name CA) (segid 3A4 and resid 350 and name CB)	11.62	0.52	0.52
	assign (segid 3A4 and resid 11 and name CA) (segid 3A4 and resid 351 and name CA)	11.90	1.07	1.06
	assign (segid 3A4 and resid 11 and name CA) (segid 3A4 and resid 352 and name CA)	9.53	1.56	1.56
	assign (segid 3A4 and resid 11 and name CA) (segid 3A4 and resid 352 and name CB)	8.58	1.63	1.63
10	assign (segid 3A4 and resid 11 and name CA) (segid 3A4 and resid 353 and name CA)	9.79	1.53	1.53
	assign (segid 3A4 and resid 11 and name CA) (segid 3A4 and resid 353 and name CB)	10.48	1.44	1.43
	assign (segid 3A4 and resid 11 and name CA) (segid 3A4 and resid 354 and name CA)	11.52	1.77	1.77
	assign (segid 3A4 and resid 11 and name CA) (segid 3A4 and resid 354 and name CB)	11.17	1.85	1.85
	assign (segid 3A4 and resid 11 and name CA) (segid 3A4 and resid 355 and name CA)	13.93	1.73	1.73
15	assign (segid 3A4 and resid 11 and name CA) (segid 3A4 and resid 355 and name CB)	13.85	1.75	1.76
	assign (segid 3A4 and resid 11 and name CA) (segid 3A4 and resid 356 and name CA)	15.13	1.54	1.54
	assign (segid 3A4 and resid 11 and name CA) (segid 3A4 and resid 356 and name CB)	14.68	1.44	1.44
	assign (segid 3A4 and resid 11 and name CA) (segid 3A4 and resid 357 and name CA)	15.05	1.71	1.70
	assign (segid 3A4 and resid 11 and name CA) (segid 3A4 and resid 357 and name CB)	14.48	1.65	1.65
20	assign (segid 3A4 and resid 11 and name CA) (segid 3A4 and resid 358 and name CA)	15.68	1.73	1.72
	assign (segid 3A4 and resid 11 and name CA) (segid 3A4 and resid 358 and name CB)	17.02	1.68	1.68
	assign (segid 3A4 and resid 11 and name CA) (segid 3A4 and resid 359 and name CA)	14.82	2.10	2.11
	assign (segid 3A4 and resid 11 and name CA) (segid 3A4 and resid 359 and name CB)	16.15	2.09	2.08
	assign (segid 3A4 and resid 11 and name CA) (segid 3A4 and resid 35 and name CA)	10.04	0.85	0.85
25	assign (segid 3A4 and resid 11 and name CA) (segid 3A4 and resid 360 and name CA)	12.55	1.91	1.91
	assign (segid 3A4 and resid 11 and name CA) (segid 3A4 and resid 360 and name CB)	11.37	1.86	1.86
	assign (segid 3A4 and resid 11 and name CA) (segid 3A4 and resid 361 and name CA)	12.40	1.95	1.95
	assign (segid 3A4 and resid 11 and name CA) (segid 3A4 and resid 361 and name CB)	11.79	1.94	1.95
	assign (segid 3A4 and resid 11 and name CA) (segid 3A4 and resid 362 and name CA)	16.14	1.94	1.93
30	assign (segid 3A4 and resid 11 and name CA) (segid 3A4 and resid 36 and name CA)	12.69	0.96	0.96
	assign (segid 3A4 and resid 11 and name CA) (segid 3A4 and resid 37 and name CA)	15.18	0.86	0.87
	assign (segid 3A4 and resid 11 and name CA) (segid 3A4 and resid 37 and name CB)	15.30	0.86	0.87
	assign (segid 3A4 and resid 11 and name CA) (segid 3A4 and resid 381 and name CA)	16.97	1.38	1.38
	assign (segid 3A4 and resid 11 and name CA) (segid 3A4 and resid 382 and name CA)	16.71	0.81	0.80
35	assign (segid 3A4 and resid 11 and name CA) (segid 3A4 and resid 382 and name CB)	15.94	0.55	0.56
	assign (segid 3A4 and resid 11 and name CA) (segid 3A4 and resid 383 and name CA)	17.18	1.24	1.24
	assign (segid 3A4 and resid 11 and name CA) (segid 3A4 and resid 38 and name CA)	14.55	0.95	0.96
	assign (segid 3A4 and resid 11 and name CA) (segid 3A4 and resid 38 and name CB)	13.56	1.11	1.10
40	assign (segid 3A4 and resid 11 and name CA) (segid 3A4 and resid 39 and name CA)	14.50	0.61	0.61
	assign (segid 3A4 and resid 11 and name CA) (segid 3A4 and resid 39 and name CB)	13.60	0.54	0.54
	assign (segid 3A4 and resid 11 and name CA) (segid 3A4 and resid 40 and name CA)	17.62	0.63	0.64
	assign (segid 3A4 and resid 11 and name CA) (segid 3A4 and resid 40 and name CB)	17.96	0.75	0.76
	assign (segid 3A4 and resid 11 and name CA) (segid 3A4 and resid 429 and name CA)	16.78	2.22	2.22
	assign (segid 3A4 and resid 11 and name CA) (segid 3A4 and resid 42 and name CA)	18.59	0.76	0.77
45	assign (segid 3A4 and resid 11 and name CA) (segid 3A4 and resid 42 and name CB)	17.38	0.81	0.81
	assign (segid 3A4 and resid 11 and name CA) (segid 3A4 and resid 430 and name CA)	16.29	0.90	0.91
	assign (segid 3A4 and resid 11 and name CA) (segid 3A4 and resid 431 and name CA)	17.44	1.44	1.45
	assign (segid 3A4 and resid 11 and name CA) (segid 3A4 and resid 433 and name CA)	16.75	2.04	2.04
	assign (segid 3A4 and resid 11 and name CB) (segid 3A4 and resid 12 and name C)	5.42	0.08	0.07
50	assign (segid 3A4 and resid 11 and name CB) (segid 3A4 and resid 12 and name CA)	4.57	0.12	0.11
	assign (segid 3A4 and resid 11 and name CB) (segid 3A4 and resid 12 and name CB)	5.52	0.20	0.21
	assign (segid 3A4 and resid 11 and name CB) (segid 3A4 and resid 12 and name N)	3.26	0.13	0.12
	assign (segid 3A4 and resid 11 and name CB) (segid 3A4 and resid 12 and name O)	6.26	0.14	0.14
	assign (segid 3A4 and resid 11 and name CB) (segid 3A4 and resid 13 and name C)	6.73	0.11	0.11
55	assign (segid 3A4 and resid 11 and name CB) (segid 3A4 and resid 13 and name CA)	6.67	0.10	0.11
	assign (segid 3A4 and resid 11 and name CB) (segid 3A4 and resid 13 and name CB)	7.11	0.18	0.18
	assign (segid 3A4 and resid 11 and name CB) (segid 3A4 and resid 13 and name N)	5.55	0.08	0.09
	assign (segid 3A4 and resid 11 and name CB) (segid 3A4 and resid 13 and name O)	7.80	0.10	0.10
	assign (segid 3A4 and resid 11 and name CB) (segid 3A4 and resid 19 and name CA)	10.26	2.00	1.99
60	assign (segid 3A4 and resid 11 and name CB) (segid 3A4 and resid 19 and name CB)	11.21	1.88	1.87
	assign (segid 3A4 and resid 11 and name CB) (segid 3A4 and resid 20 and name CA)	12.38	2.05	2.04
	assign (segid 3A4 and resid 11 and name CB) (segid 3A4 and resid 20 and name CB)	13.74	1.98	1.99
	assign (segid 3A4 and resid 11 and name CB) (segid 3A4 and resid 21 and name CA)	12.65	2.24	2.25
	assign (segid 3A4 and resid 11 and name CB) (segid 3A4 and resid 21 and name CB)	11.59	2.27	2.28
65	assign (segid 3A4 and resid 11 and name CB) (segid 3A4 and resid 22 and name CA)	14.94	2.26	2.26
	assign (segid 3A4 and resid 11 and name CB) (segid 3A4 and resid 23 and name CA)	14.62	1.96	1.96
	assign (segid 3A4 and resid 11 and name CB) (segid 3A4 and resid 23 and name CB)	13.62	1.85	1.84
	assign (segid 3A4 and resid 11 and name CB) (segid 3A4 and resid 30 and name CA)	17.32	1.93	1.93
	assign (segid 3A4 and resid 11 and name CB) (segid 3A4 and resid 314 and name CA)	15.23	1.70	1.71
70	assign (segid 3A4 and resid 11 and name CB) (segid 3A4 and resid 314 and name CB)	15.56	1.67	1.68
	assign (segid 3A4 and resid 11 and name CB) (segid 3A4 and resid 315 and name CA)	13.76	2.17	2.16
	assign (segid 3A4 and resid 11 and name CB) (segid 3A4 and resid 315 and name CB)	14.63	2.29	2.30
	assign (segid 3A4 and resid 11 and name CB) (segid 3A4 and resid 316 and name CA)	14.29	2.35	2.35
	assign (segid 3A4 and resid 11 and name CB) (segid 3A4 and resid 317 and name CA)	14.03	1.70	1.70
75	assign (segid 3A4 and resid 11 and name CB) (segid 3A4 and resid 318 and name CA)	16.09	2.18	2.19
	assign (segid 3A4 and resid 11 and name CB) (segid 3A4 and resid 319 and name CA)	16.10	1.91	1.91
	assign (segid 3A4 and resid 11 and name CB) (segid 3A4 and resid 319 and name CB)	17.15	1.80	1.80
	assign (segid 3A4 and resid 11 and name CB) (segid 3A4 and resid 31 and name CA)	15.26	1.92	1.91
	assign (segid 3A4 and resid 11 and name CB) (segid 3A4 and resid 31 and name CB)	16.06	1.91	1.90
80	assign (segid 3A4 and resid 11 and name CB) (segid 3A4 and resid 32 and name CA)	11.92	1.77	1.77
	assign (segid 3A4 and resid 11 and name CB) (segid 3A4 and resid 32 and name CB)	10.84	1.76	1.76
	assign (segid 3A4 and resid 11 and name CB) (segid 3A4 and resid 33 and name CA)	11.67	1.60	1.59

	assign	(segid 3A4 and resid 11 and name CB)	(segid 3A4 and resid 33 and name CB)	12.85	1.50	1.50
	assign	(segid 3A4 and resid 11 and name CB)	(segid 3A4 and resid 343 and name CA)	17.27	1.72	1.73
	assign	(segid 3A4 and resid 11 and name CB)	(segid 3A4 and resid 343 and name CB)	17.61	1.69	1.69
	assign	(segid 3A4 and resid 11 and name CB)	(segid 3A4 and resid 344 and name CA)	14.67	1.62	1.62
5	assign	(segid 3A4 and resid 11 and name CB)	(segid 3A4 and resid 344 and name CB)	14.04	1.54	1.55
	assign	(segid 3A4 and resid 11 and name CB)	(segid 3A4 and resid 345 and name CA)	13.43	1.63	1.62
	assign	(segid 3A4 and resid 11 and name CB)	(segid 3A4 and resid 345 and name CB)	14.54	1.63	1.63
	assign	(segid 3A4 and resid 11 and name CB)	(segid 3A4 and resid 346 and name CA)	10.57	1.59	1.59
	assign	(segid 3A4 and resid 11 and name CB)	(segid 3A4 and resid 346 and name CB)	9.31	1.55	1.55
10	assign	(segid 3A4 and resid 11 and name CB)	(segid 3A4 and resid 347 and name CA)	12.13	1.37	1.38
	assign	(segid 3A4 and resid 11 and name CB)	(segid 3A4 and resid 347 and name CB)	13.38	1.46	1.47
	assign	(segid 3A4 and resid 11 and name CB)	(segid 3A4 and resid 348 and name CA)	9.88	1.51	1.51
	assign	(segid 3A4 and resid 11 and name CB)	(segid 3A4 and resid 349 and name CA)	7.62	0.72	0.73
	assign	(segid 3A4 and resid 11 and name CB)	(segid 3A4 and resid 349 and name CB)	7.22	0.67	0.66
15	assign	(segid 3A4 and resid 11 and name CB)	(segid 3A4 and resid 34 and name CA)	8.83	1.07	1.07
	assign	(segid 3A4 and resid 11 and name CB)	(segid 3A4 and resid 34 and name CB)	7.80	1.26	1.26
	assign	(segid 3A4 and resid 11 and name CB)	(segid 3A4 and resid 350 and name CA)	10.50	0.34	0.33
	assign	(segid 3A4 and resid 11 and name CB)	(segid 3A4 and resid 350 and name CB)	11.66	0.41	0.41
	assign	(segid 3A4 and resid 11 and name CB)	(segid 3A4 and resid 351 and name CA)	11.55	0.96	0.95
20	assign	(segid 3A4 and resid 11 and name CB)	(segid 3A4 and resid 352 and name CA)	9.07	1.49	1.49
	assign	(segid 3A4 and resid 11 and name CB)	(segid 3A4 and resid 352 and name CB)	8.07	1.58	1.57
	assign	(segid 3A4 and resid 11 and name CB)	(segid 3A4 and resid 353 and name CA)	9.66	1.33	1.34
	assign	(segid 3A4 and resid 11 and name CB)	(segid 3A4 and resid 353 and name CB)	10.47	1.16	1.16
	assign	(segid 3A4 and resid 11 and name CB)	(segid 3A4 and resid 354 and name CA)	11.23	1.74	1.74
25	assign	(segid 3A4 and resid 11 and name CB)	(segid 3A4 and resid 354 and name CB)	10.88	1.86	1.86
	assign	(segid 3A4 and resid 11 and name CB)	(segid 3A4 and resid 355 and name CA)	13.86	1.55	1.54
	assign	(segid 3A4 and resid 11 and name CB)	(segid 3A4 and resid 355 and name CB)	13.91	1.54	1.54
	assign	(segid 3A4 and resid 11 and name CB)	(segid 3A4 and resid 356 and name CA)	14.93	1.37	1.38
	assign	(segid 3A4 and resid 11 and name CB)	(segid 3A4 and resid 356 and name CB)	14.52	1.27	1.28
30	assign	(segid 3A4 and resid 11 and name CB)	(segid 3A4 and resid 357 and name CA)	14.57	1.67	1.67
	assign	(segid 3A4 and resid 11 and name CB)	(segid 3A4 and resid 357 and name CB)	13.95	1.61	1.61
	assign	(segid 3A4 and resid 11 and name CB)	(segid 3A4 and resid 358 and name CA)	15.09	1.88	1.87
	assign	(segid 3A4 and resid 11 and name CB)	(segid 3A4 and resid 358 and name CB)	16.44	1.85	1.84
	assign	(segid 3A4 and resid 11 and name CB)	(segid 3A4 and resid 359 and name CA)	14.01	2.35	2.35
35	assign	(segid 3A4 and resid 11 and name CB)	(segid 3A4 and resid 359 and name CB)	15.29	2.36	2.36
	assign	(segid 3A4 and resid 11 and name CB)	(segid 3A4 and resid 35 and name CA)	10.57	0.93	0.93
	assign	(segid 3A4 and resid 11 and name CB)	(segid 3A4 and resid 360 and name CA)	11.77	2.08	2.08
	assign	(segid 3A4 and resid 11 and name CB)	(segid 3A4 and resid 360 and name CB)	10.68	1.99	1.99
40	assign	(segid 3A4 and resid 11 and name CB)	(segid 3A4 and resid 361 and name CA)	11.41	2.23	2.23
	assign	(segid 3A4 and resid 11 and name CB)	(segid 3A4 and resid 361 and name CB)	10.77	2.26	2.26
	assign	(segid 3A4 and resid 11 and name CB)	(segid 3A4 and resid 362 and name CA)	15.13	2.22	2.22
	assign	(segid 3A4 and resid 11 and name CB)	(segid 3A4 and resid 36 and name CA)	12.97	0.88	0.88
	assign	(segid 3A4 and resid 11 and name CB)	(segid 3A4 and resid 37 and name CA)	15.62	0.95	0.96
	assign	(segid 3A4 and resid 11 and name CB)	(segid 3A4 and resid 37 and name CB)	15.78	0.97	0.96
45	assign	(segid 3A4 and resid 11 and name CB)	(segid 3A4 and resid 381 and name CA)	16.68	1.27	1.27
	assign	(segid 3A4 and resid 11 and name CB)	(segid 3A4 and resid 382 and name CA)	16.57	0.68	0.69
	assign	(segid 3A4 and resid 11 and name CB)	(segid 3A4 and resid 382 and name CB)	15.91	0.39	0.38
	assign	(segid 3A4 and resid 11 and name CB)	(segid 3A4 and resid 383 and name CA)	16.91	1.25	1.24

	assign (segid 3A4 and resid 120 and name C)	(segid 3A4 and resid 120 and name CB)	2.49	0.04	0.03
	assign (segid 3A4 and resid 120 and name C)	(segid 3A4 and resid 120 and name O)	1.24	0.02	0.02
	assign (segid 3A4 and resid 120 and name C)	(segid 3A4 and resid 121 and name C)	3.04	0.06	0.07
	assign (segid 3A4 and resid 120 and name C)	(segid 3A4 and resid 121 and name CA)	2.43	0.02	0.02
	assign (segid 3A4 and resid 120 and name C)	(segid 3A4 and resid 121 and name CB)	3.69	0.04	0.04
5	assign (segid 3A4 and resid 120 and name C)	(segid 3A4 and resid 121 and name N)	1.32	0.03	0.02
	assign (segid 3A4 and resid 120 and name C)	(segid 3A4 and resid 121 and name O)	3.99	0.13	0.13
	assign (segid 3A4 and resid 120 and name C)	(segid 3A4 and resid 122 and name C)	4.68	0.21	0.21
	assign (segid 3A4 and resid 120 and name C)	(segid 3A4 and resid 122 and name CA)	4.42	0.18	0.19
	assign (segid 3A4 and resid 120 and name C)	(segid 3A4 and resid 122 and name CB)	5.11	0.24	0.23
10	assign (segid 3A4 and resid 120 and name C)	(segid 3A4 and resid 122 and name N)	3.19	0.20	0.20
	assign (segid 3A4 and resid 120 and name C)	(segid 3A4 and resid 122 and name O)	5.67	0.30	0.30
	assign (segid 3A4 and resid 120 and name C)	(segid 3A4 and resid 123 and name C)	5.28	0.44	0.44
	assign (segid 3A4 and resid 120 and name C)	(segid 3A4 and resid 123 and name CA)	5.05	0.28	0.28
	assign (segid 3A4 and resid 120 and name C)	(segid 3A4 and resid 123 and name CB)	5.16	0.34	0.34
15	assign (segid 3A4 and resid 120 and name C)	(segid 3A4 and resid 123 and name N)	4.18	0.19	0.19
	assign (segid 3A4 and resid 120 and name C)	(segid 3A4 and resid 123 and name O)	6.44	0.40	0.41
	assign (segid 3A4 and resid 120 and name C)	(segid 3A4 and resid 124 and name C)	6.02	0.65	0.64
	assign (segid 3A4 and resid 120 and name C)	(segid 3A4 and resid 124 and name CA)	5.28	0.70	0.70
	assign (segid 3A4 and resid 120 and name C)	(segid 3A4 and resid 124 and name CB)	4.86	0.78	0.78
20	assign (segid 3A4 and resid 120 and name C)	(segid 3A4 and resid 124 and name N)	4.50	0.61	0.60
	assign (segid 3A4 and resid 120 and name C)	(segid 3A4 and resid 125 and name CA)	6.85	0.43	0.42
	assign (segid 3A4 and resid 120 and name C)	(segid 3A4 and resid 125 and name CB)	6.64	0.38	0.38
	assign (segid 3A4 and resid 120 and name C)	(segid 3A4 and resid 125 and name N)	5.77	0.47	0.48
	assign (segid 3A4 and resid 120 and name C)	(segid 3A4 and resid 125 and name O)	4.93	0.48	0.49
25	assign (segid 3A4 and resid 120 and name C)	(segid 3A4 and resid 438 and name C)	5.87	0.63	0.63
	assign (segid 3A4 and resid 120 and name C)	(segid 3A4 and resid 438 and name CA)	5.70	0.72	0.73
	assign (segid 3A4 and resid 120 and name C)	(segid 3A4 and resid 438 and name N)	3.92	0.42	0.42
	assign (segid 3A4 and resid 120 and name C)	(segid 3A4 and resid 438 and name O)	6.04	0.23	0.23
	assign (segid 3A4 and resid 120 and name C)	(segid 3A4 and resid 439 and name C)	5.37	0.21	0.21
30	assign (segid 3A4 and resid 120 and name C)	(segid 3A4 and resid 439 and name CA)	5.57	0.39	0.40
	assign (segid 3A4 and resid 120 and name C)	(segid 3A4 and resid 439 and name N)	7.13	0.24	0.24
	assign (segid 3A4 and resid 120 and name C)	(segid 3A4 and resid 439 and name O)	7.24	0.17	0.18
	assign (segid 3A4 and resid 120 and name C)	(segid 3A4 and resid 440 and name C)	6.73	0.27	0.28
	assign (segid 3A4 and resid 120 and name C)	(segid 3A4 and resid 440 and name CA)	5.70	0.26	0.26
35	assign (segid 3A4 and resid 120 and name C)	(segid 3A4 and resid 440 and name N)	6.71	0.13	0.14
	assign (segid 3A4 and resid 120 and name C)	(segid 3A4 and resid 440 and name O)	1.52	0.01	0.01
	assign (segid 3A4 and resid 120 and name CA)	(segid 3A4 and resid 120 and name CB)	1.50	0.02	0.02
	assign (segid 3A4 and resid 120 and name CA)	(segid 3A4 and resid 120 and name O)	2.38	0.02	0.02
40	assign (segid 3A4 and resid 120 and name CA)	(segid 3A4 and resid 121 and name C)	4.48	0.05	0.04
	assign (segid 3A4 and resid 120 and name CA)	(segid 3A4 and resid 121 and name CB)	3.81	0.02	0.02
	assign (segid 3A4 and resid 120 and name CA)	(segid 3A4 and resid 121 and name N)	4.83	0.05	0.06
	assign (segid 3A4 and resid 120 and name CA)	(segid 3A4 and resid 121 and name O)	2.44	0.02	0.01
	assign (segid 3A4 and resid 120 and name CA)	(segid 3A4 and resid 121 and name CB)	5.47	0.11	0.11
45	assign (segid 3A4 and resid 120 and name CA)	(segid 3A4 and resid 122 and name C)	5.79	0.25	0.25
	assign (segid 3A4 and resid 120 and name CA)	(segid 3A4 and resid 122 and name CA)	5.53	0.23	0.23
	assign (segid 3A4 and resid 120 and name CA)	(segid 3A4 and resid 122 and name CB)	5.91	0.33	0.32
	assign (segid 3A4 and resid 120 and name CA)	(segid 3A4 and resid 122 and name N)	4.39	0.22	0.21
	assign (segid 3A4 and resid 120 and name CA)	(segid 3A4 and resid 122 and name O)	6.85	0.32	0.32
50	assign (segid 3A4 and resid 120 and name CA)	(segid 3A4 and resid 123 and name C)	6.21	0.60	0.60
	assign (segid 3A4 and resid 120 and name CA)	(segid 3A4 and resid 123 and name CA)	5.85	0.43	0.42
	assign (segid 3A4 and resid 120 and name CA)	(segid 3A4 and resid 123 and name CB)	5.60	0.51	0.51
	assign (segid 3A4 and resid 120 and name CA)	(segid 3A4 and resid 123 and name N)	5.10	0.29	0.29
	assign (segid 3A4 and resid 120 and name CA)	(segid 3A4 and resid 124 and name CA)	6.35	0.86	0.86
55	assign (segid 3A4 and resid 120 and name CA)	(segid 3A4 and resid 124 and name CB)	5.81	0.97	0.98
	assign (segid 3A4 and resid 120 and name CA)	(segid 3A4 and resid 124 and name N)	5.54	0.75	0.75
	assign (segid 3A4 and resid 120 and name CA)	(segid 3A4 and resid 125 and name CA)	8.28	0.44	0.44
	assign (segid 3A4 and resid 120 and name CA)	(segid 3A4 and resid 125 and name CB)	8.09	0.39	0.39
	assign (segid 3A4 and resid 120 and name CA)	(segid 3A4 and resid 125 and name N)	9.72	0.69	0.69
	assign (segid 3A4 and resid 120 and name CA)	(segid 3A4 and resid 126 and name CA)	10.77	0.79	0.79
60	assign (segid 3A4 and resid 120 and name CA)	(segid 3A4 and resid 127 and name CA)	10.18	0.80	0.80
	assign (segid 3A4 and resid 120 and name CA)	(segid 3A4 and resid 128 and name CA)	12.50	0.78	0.79
	assign (segid 3A4 and resid 120 and name CA)	(segid 3A4 and resid 128 and name CB)	12.01	0.84	0.84
	assign (segid 3A4 and resid 120 and name CA)	(segid 3A4 and resid 129 and name CA)	14.26	0.81	0.80
	assign (segid 3A4 and resid 120 and name CA)	(segid 3A4 and resid 129 and name CB)	13.83	0.78	0.77
65	assign (segid 3A4 and resid 120 and name CA)	(segid 3A4 and resid 130 and name CA)	16.14	0.46	0.46
	assign (segid 3A4 and resid 120 and name CA)	(segid 3A4 and resid 130 and name CB)	15.70	0.38	0.38
	assign (segid 3A4 and resid 120 and name CA)	(segid 3A4 and resid 131 and name CA)	16.99	0.76	0.77
	assign (segid 3A4 and resid 120 and name CA)	(segid 3A4 and resid 131 and name CB)	16.23	0.85	0.84
70	assign (segid 3A4 and resid 120 and name CA)	(segid 3A4 and resid 150 and name CA)	18.54	1.01	1.01
	assign (segid 3A4 and resid 120 and name CA)	(segid 3A4 and resid 256 and name CA)	17.59	0.41	0.41
	assign (segid 3A4 and resid 120 and name CA)	(segid 3A4 and resid 257 and name CA)	16.27	0.65	0.65
	assign (segid 3A4 and resid 120 and name CA)	(segid 3A4 and resid 258 and name CA)	17.63	0.32	0.33
	assign (segid 3A4 and resid 120 and name CA)	(segid 3A4 and resid 258 and name CB)	19.13	0.31	0.31
	assign (segid 3A4 and resid 120 and name CA)	(segid 3A4 and resid 259 and name CA)	16.33	0.21	0.20
75	assign (segid 3A4 and resid 120 and name CA)	(segid 3A4 and resid 259 and name CB)	16.85	0.22	0.22
	assign (segid 3A4 and resid 120 and name CA)	(segid 3A4 and resid 260 and name CA)	12.70	0.29	0.29
	assign (segid 3A4 and resid 120 and name CA)	(segid 3A4 and resid 260 and name CB)	12.36	0.47	0.46
	assign (segid 3A4 and resid 120 and name CA)	(segid 3A4 and resid 261 and name CA)	13.08	0.41	0.41
	assign (segid 3A4 and resid 120 and name CA)	(segid 3A4 and resid 262 and name CA)	14.97	0.33	0.32
80	assign (segid 3A4 and resid 120 and name CA)	(segid 3A4 and resid 262 and name CB)	16.20	0.27	0.27
	assign (segid 3A4 and resid 120 and name CA)	(segid 3A4 and resid 263 and name CA)	12.56	0.13	0.14
	assign (segid 3A4 and resid 120 and name CA)	(segid 3A4 and resid 263 and name CB)	12.15	0.11	0.12

	assign (segid 3A4 and resid 120 and name CA) (segid 3A4 and resid 264 and name CA)	9.87	0.27	0.27
	assign (segid 3A4 and resid 120 and name CA) (segid 3A4 and resid 265 and name CA)	12.93	0.38	0.38
	assign (segid 3A4 and resid 120 and name CA) (segid 3A4 and resid 266 and name CA)	14.22	0.33	0.34
	assign (segid 3A4 and resid 120 and name CA) (segid 3A4 and resid 267 and name CA)	11.46	0.35	0.36
	assign (segid 3A4 and resid 120 and name CA) (segid 3A4 and resid 267 and name CB)	10.11	0.34	0.33
5	assign (segid 3A4 and resid 120 and name CA) (segid 3A4 and resid 268 and name CA)	11.73	0.44	0.44
	assign (segid 3A4 and resid 120 and name CA) (segid 3A4 and resid 268 and name CB)	11.71	0.40	0.41
	assign (segid 3A4 and resid 120 and name CA) (segid 3A4 and resid 269 and name CA)	15.44	0.44	0.44
	assign (segid 3A4 and resid 120 and name CA) (segid 3A4 and resid 270 and name CA)	15.63	0.54	0.55
	assign (segid 3A4 and resid 120 and name CA) (segid 3A4 and resid 270 and name CB)	15.29	0.52	0.51
10	assign (segid 3A4 and resid 120 and name CA) (segid 3A4 and resid 271 and name CA)	13.76	0.68	0.67
	assign (segid 3A4 and resid 120 and name CA) (segid 3A4 and resid 271 and name CB)	12.34	0.67	0.67
	assign (segid 3A4 and resid 120 and name CA) (segid 3A4 and resid 272 and name CA)	16.25	0.63	0.62
	assign (segid 3A4 and resid 120 and name CA) (segid 3A4 and resid 272 and name CB)	16.30	0.59	0.60
	assign (segid 3A4 and resid 120 and name CA) (segid 3A4 and resid 277 and name CA)	19.23	0.42	0.42
15	assign (segid 3A4 and resid 120 and name CA) (segid 3A4 and resid 277 and name CB)	18.13	0.43	0.43
	assign (segid 3A4 and resid 120 and name CA) (segid 3A4 and resid 312 and name CB)	18.65	0.79	0.79
	assign (segid 3A4 and resid 120 and name CA) (segid 3A4 and resid 318 and name CB)	18.58	0.66	0.66
	assign (segid 3A4 and resid 120 and name CA) (segid 3A4 and resid 400 and name CB)	18.94	0.42	0.41
20	assign (segid 3A4 and resid 120 and name CA) (segid 3A4 and resid 401 and name CA)	18.03	0.35	0.35
	assign (segid 3A4 and resid 120 and name CA) (segid 3A4 and resid 404 and name CA)	16.04	0.46	0.46
	assign (segid 3A4 and resid 120 and name CA) (segid 3A4 and resid 404 and name CB)	15.15	0.41	0.41
	assign (segid 3A4 and resid 120 and name CA) (segid 3A4 and resid 405 and name CA)	16.32	0.56	0.56
	assign (segid 3A4 and resid 120 and name CA) (segid 3A4 and resid 405 and name CB)	16.87	0.55	0.56
	assign (segid 3A4 and resid 120 and name CA) (segid 3A4 and resid 407 and name CA)	17.72	0.58	0.58
25	assign (segid 3A4 and resid 120 and name CA) (segid 3A4 and resid 407 and name CB)	17.60	0.66	0.66
	assign (segid 3A4 and resid 120 and name CA) (segid 3A4 and resid 408 and name CA)	14.42	0.57	0.56
	assign (segid 3A4 and resid 120 and name CA) (segid 3A4 and resid 408 and name CB)	13.36	0.46	0.46
	assign (segid 3A4 and resid 120 and name CA) (segid 3A4 and resid 409 and name CA)	16.42	0.49	0.48
	assign (segid 3A4 and resid 120 and name CA) (segid 3A4 and resid 409 and name CB)	17.09	0.53	0.53
30	assign (segid 3A4 and resid 120 and name CA) (segid 3A4 and resid 409 and name CB)	19.07	0.44	0.43
	assign (segid 3A4 and resid 120 and name CA) (segid 3A4 and resid 410 and name CA)	16.98	0.49	0.49
	assign (segid 3A4 and resid 120 and name CA) (segid 3A4 and resid 411 and name CA)	16.26	0.62	0.62
	assign (segid 3A4 and resid 120 and name CA) (segid 3A4 and resid 411 and name CB)	14.89	0.33	0.32
	assign (segid 3A4 and resid 120 and name CA) (segid 3A4 and resid 412 and name CA)	15.03	0.92	0.92
35	assign (segid 3A4 and resid 120 and name CA) (segid 3A4 and resid 413 and name CA)	12.19	0.30	0.31
	assign (segid 3A4 and resid 120 and name CA) (segid 3A4 and resid 414 and name CA)	11.62	0.74	0.74
	assign (segid 3A4 and resid 120 and name CA) (segid 3A4 and resid 415 and name CA)	12.45	0.78	0.78
	assign (segid 3A4 and resid 120 and name CA) (segid 3A4 and resid 415 and name CB)	10.27	0.68	0.68
40	assign (segid 3A4 and resid 120 and name CA) (segid 3A4 and resid 416 and name CA)	10.90	1.27	1.26
	assign (segid 3A4 and resid 120 and name CA) (segid 3A4 and resid 417 and name CA)	12.89	1.37	1.37
	assign (segid 3A4 and resid 120 and name CA) (segid 3A4 and resid 423 and name CA)	12.51	1.48	1.49
	assign (segid 3A4 and resid 120 and name CA) (segid 3A4 and resid 424 and name CA)	12.94	1.82	1.82
	assign (segid 3A4 and resid 120 and name CA) (segid 3A4 and resid 425 and name CA)	14.28	1.06	1.06
	assign (segid 3A4 and resid 120 and name CA) (segid 3A4 and resid 426 and name CA)	15.52	0.84	0.84
45	assign (segid 3A4 and resid 120 and name CA) (segid 3A4 and resid 427 and name CA)	17.89	1.42	1.43
	assign (segid 3A4 and resid 120 and name CA) (segid 3A4 and resid 428 and name CA)	17.56	0.60	0.60
	assign (segid 3A4 and resid 120 and name CA) (segid 3A4 and resid 433 and name CA)	14.07	0.64	0.64
	assign (segid 3A4 and resid 120 and name CA) (segid 3A4 and resid 434 and name CA)	11.17	0.48	0.49
	assign (segid 3A4 and resid 120 and name CA) (segid 3A4 and resid 435 and name CA)	9.86	0.59	0.59
50	assign (segid 3A4 and resid 120 and name CA) (segid 3A4 and resid 436 and name CA)	6.40	0.50	0.50
	assign (segid 3A4 and resid 120 and name CA) (segid 3A4 and resid 437 and name CA)	6.66	0.58	0.59
	assign (segid 3A4 and resid 120 and name CA) (segid 3A4 and resid 438 and name CA)	4.55	0.33	0.33
	assign (segid 3A4 and resid 120 and name CA) (segid 3A4 and resid 438 and name CB)	5.65	0.44	0.45
	assign (segid 3A4 and resid 120 and name CA) (segid 3A4 and resid 438 and name N)	5.46	0.58	0.59
55	assign (segid 3A4 and resid 120 and name CA) (segid 3A4 and resid 438 and name O)	3.73	0.22	0.22
	assign (segid 3A4 and resid 120 and name CA) (segid 3A4 and resid 439 and name C)	5.41	0.22	0.22
	assign (segid 3A4 and resid 120 and name CA) (segid 3A4 and resid 439 and name CA)	4.52	0.18	0.18
	assign (segid 3A4 and resid 120 and name CA) (segid 3A4 and resid 439 and name N)	4.89	0.32	0.32
	assign (segid 3A4 and resid 120 and name CA) (segid 3A4 and resid 439 and name O)	6.56	0.22	0.22
60	assign (segid 3A4 and resid 120 and name CA) (segid 3A4 and resid 440 and name C)	6.85	0.17	0.18
	assign (segid 3A4 and resid 120 and name CA) (segid 3A4 and resid 440 and name CA)	6.41	0.26	0.26
	assign (segid 3A4 and resid 120 and name CA) (segid 3A4 and resid 440 and name N)	5.20	0.25	0.25
	assign (segid 3A4 and resid 120 and name CA) (segid 3A4 and resid 440 and name O)	6.22	0.13	0.13
	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 121 and name C)	5.11	0.10	0.09
65	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 121 and name CA)	4.83	0.06	0.06
	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 121 and name CB)	5.98	0.09	0.09
	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 121 and name N)	3.58	0.04	0.05
	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 121 and name O)	6.04	0.14	0.15
	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 122 and name C)	5.61	0.33	0.33
70	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 122 and name CA)	5.55	0.31	0.30
	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 122 and name CB)	5.68	0.46	0.45
	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 122 and name N)	4.72	0.27	0.27
	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 122 and name O)	6.70	0.37	0.37
	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 123 and name C)	5.88	0.77	0.77
75	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 123 and name CA)	5.29	0.59	0.59
	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 123 and name CB)	4.75	0.73	0.73
	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 123 and name N)	4.71	0.42	0.42
	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 124 and name CA)	6.50	0.96	0.97
	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 124 and name CB)	6.20	1.06	1.06
80	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 124 and name N)	5.49	0.89	0.88
	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 125 and name CA)	8.74	0.49	0.49
	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 125 and name CB)	8.75	0.35	0.36

	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 126 and name CA)	9.90	0.61	0.61
	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 127 and name CA)	10.57	0.94	0.94
	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 127 and name CB)	9.85	1.03	1.03
	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 128 and name CA)	12.50	0.98	0.99
5	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 128 and name CB)	12.10	1.05	1.04
	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 129 and name CA)	14.46	0.84	0.84
	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 129 and name CB)	14.14	0.75	0.75
	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 130 and name CA)	16.13	0.51	0.52
10	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 130 and name CB)	15.64	0.47	0.47
	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 131 and name CA)	16.82	0.91	0.91
	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 131 and name CB)	16.00	1.04	1.04
	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 150 and name CA)	17.83	0.97	0.97
	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 154 and name CA)	16.54	1.28	1.29
15	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 157 and name CB)	17.65	1.33	1.32
	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 256 and name CA)	17.33	0.42	0.43
	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 257 and name CA)	15.95	0.69	0.69
	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 258 and name CA)	17.57	0.37	0.38
	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 258 and name CB)	19.09	0.37	0.37
20	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 259 and name CA)	16.51	0.28	0.29
	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 259 and name CB)	17.04	0.32	0.33
	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 260 and name CA)	12.80	0.35	0.35
	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 260 and name CB)	12.29	0.52	0.51
	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 261 and name CA)	13.17	0.42	0.42
25	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 262 and name CA)	15.38	0.31	0.31
	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 262 and name CB)	16.62	0.25	0.25
	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 263 and name CA)	13.22	0.15	0.15
	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 263 and name CB)	12.79	0.20	0.19
	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 264 and name CA)	10.47	0.26	0.25
30	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 265 and name CA)	13.52	0.37	0.37
	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 266 and name CA)	15.11	0.34	0.34
	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 267 and name CA)	12.57	0.38	0.37
	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 267 and name CB)	11.23	0.36	0.36
	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 268 and name CA)	12.66	0.46	0.46
35	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 268 and name CB)	12.49	0.43	0.44
	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 269 and name CA)	16.40	0.45	0.46
	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 270 and name CA)	16.83	0.55	0.55
	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 270 and name CB)	16.53	0.51	0.50
	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 271 and name CA)	14.98	0.70	0.69
40	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 271 and name CB)	13.54	0.69	0.69
	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 272 and name CA)	17.30	0.64	0.63
	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 272 and name CB)	17.27	0.60	0.60
	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 318 and name CB)	18.65	0.68	0.68
	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 401 and name CA)	18.78	0.40	0.40
45	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 404 and name CA)	16.98	0.49	0.49
	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 404 and name CB)	16.02	0.44	0.43
	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 405 and name CA)	17.44	0.58	0.57
	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 405 and name CB)	17.97	0.59	0.58
	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 407 and name CA)	18.89	0.61	0.62
50	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 408 and name CA)	15.68	0.58	0.59
	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 408 and name CB)	14.62	0.47	0.47
	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 409 and name CA)	17.80	0.49	0.49
	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 409 and name CB)	18.46	0.52	0.53
	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 411 and name CA)	18.32	0.51	0.51
55	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 411 and name CB)	17.56	0.65	0.64
	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 412 and name CA)	16.32	0.33	0.33
	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 413 and name CA)	16.49	0.96	0.97
	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 414 and name CA)	13.62	0.36	0.35
	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 415 and name CA)	12.90	0.87	0.88
60	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 415 and name CB)	13.70	0.95	0.94
	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 416 and name CA)	11.33	0.79	0.79
	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 417 and name CA)	11.74	1.17	1.16
	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 423 and name CA)	13.12	1.39	1.40
	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 424 and name CA)	12.70	1.64	1.64
65	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 425 and name CA)	12.85	2.00	2.00
	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 426 and name CA)	14.05	1.16	1.17
	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 427 and name CA)	15.11	0.82	0.82
	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 428 and name CA)	17.35	1.31	1.31
	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 433 and name CA)	17.34	0.59	0.60
70	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 434 and name CA)	13.91	0.52	0.51
	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 435 and name CA)	11.09	0.49	0.49
	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 436 and name CA)	9.35	0.72	0.72
	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 437 and name C)	6.27	0.57	0.56
	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 437 and name CA)	6.23	0.71	0.70
75	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 438 and name C)	5.20	0.35	0.35
	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 438 and name CA)	6.08	0.49	0.49
	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 438 and name N)	5.56	0.67	0.67
	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 438 and name O)	4.56	0.23	0.23
	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 439 and name C)	6.45	0.29	0.29
80	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 439 and name CA)	5.33	0.28	0.27
	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 439 and name N)	5.52	0.41	0.42
	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 440 and name CA)	7.73	0.28	0.28
	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 440 and name N)	6.43	0.29	0.28
	assign (segid 3A4 and resid 120 and name CB) (segid 3A4 and resid 440 and name O)	7.49	0.16	0.16

	assign (segid 3A4 and resid 120 and name N) (segid 3A4 and resid 120 and name C)	2.33	0.02	0.03
	assign (segid 3A4 and resid 120 and name N) (segid 3A4 and resid 120 and name CA)	1.45	0.00	0.01
	assign (segid 3A4 and resid 120 and name N) (segid 3A4 and resid 120 and name CB)	2.45	0.04	0.03
5	assign (segid 3A4 and resid 120 and name N) (segid 3A4 and resid 120 and name O)	2.88	0.04	0.04
	assign (segid 3A4 and resid 120 and name N) (segid 3A4 and resid 121 and name C)	5.32	0.08	0.08
	assign (segid 3A4 and resid 120 and name N) (segid 3A4 and resid 121 and name CA)	4.43	0.07	0.06
	assign (segid 3A4 and resid 120 and name N) (segid 3A4 and resid 121 and name CB)	5.43	0.06	0.06
	assign (segid 3A4 and resid 120 and name N) (segid 3A4 and resid 121 and name N)	3.19	0.06	0.06
	assign (segid 3A4 and resid 120 and name N) (segid 3A4 and resid 121 and name O)	6.17	0.18	0.18
10	assign (segid 3A4 and resid 120 and name N) (segid 3A4 and resid 122 and name C)	6.79	0.27	0.28
	assign (segid 3A4 and resid 120 and name N) (segid 3A4 and resid 122 and name CA)	6.68	0.20	0.20
	assign (segid 3A4 and resid 120 and name N) (segid 3A4 and resid 122 and name CB)	7.21	0.30	0.30
	assign (segid 3A4 and resid 120 and name N) (segid 3A4 and resid 122 and name N)	5.50	0.20	0.20
	assign (segid 3A4 and resid 120 and name N) (segid 3A4 and resid 123 and name CA)	6.60	0.41	0.40
15	assign (segid 3A4 and resid 120 and name N) (segid 3A4 and resid 123 and name CB)	6.28	0.43	0.43
	assign (segid 3A4 and resid 120 and name N) (segid 3A4 and resid 123 and name N)	6.06	0.27	0.26
	assign (segid 3A4 and resid 120 and name N) (segid 3A4 and resid 124 and name N)	5.86	0.80	0.80
	assign (segid 3A4 and resid 120 and name N) (segid 3A4 and resid 438 and name C)	5.46	0.24	0.25
	assign (segid 3A4 and resid 120 and name N) (segid 3A4 and resid 438 and name CA)	6.73	0.35	0.35
20	assign (segid 3A4 and resid 120 and name N) (segid 3A4 and resid 438 and name N)	6.71	0.50	0.50
	assign (segid 3A4 and resid 120 and name N) (segid 3A4 and resid 438 and name O)	4.64	0.18	0.19
	assign (segid 3A4 and resid 120 and name N) (segid 3A4 and resid 439 and name C)	5.54	0.14	0.13
	assign (segid 3A4 and resid 120 and name N) (segid 3A4 and resid 439 and name CA)	4.86	0.10	0.10
	assign (segid 3A4 and resid 120 and name N) (segid 3A4 and resid 439 and name N)	5.58	0.20	0.21
25	assign (segid 3A4 and resid 120 and name N) (segid 3A4 and resid 439 and name O)	6.75	0.14	0.14
	assign (segid 3A4 and resid 120 and name N) (segid 3A4 and resid 440 and name C)	6.27	0.13	0.14
	assign (segid 3A4 and resid 120 and name N) (segid 3A4 and resid 440 and name CA)	6.14	0.17	0.17
	assign (segid 3A4 and resid 120 and name N) (segid 3A4 and resid 440 and name N)	5.06	0.17	0.16
	assign (segid 3A4 and resid 120 and name N) (segid 3A4 and resid 440 and name O)	5.46	0.15	0.15
30	assign (segid 3A4 and resid 120 and name O) (segid 3A4 and resid 120 and name CB)	2.86	0.05	0.04
	assign (segid 3A4 and resid 120 and name O) (segid 3A4 and resid 121 and name C)	2.98	0.08	0.07
	assign (segid 3A4 and resid 120 and name O) (segid 3A4 and resid 121 and name CA)	2.78	0.02	0.02
	assign (segid 3A4 and resid 120 and name O) (segid 3A4 and resid 121 and name CB)	4.26	0.01	0.02
	assign (segid 3A4 and resid 120 and name O) (segid 3A4 and resid 121 and name N)	2.24	0.01	0.02
35	assign (segid 3A4 and resid 120 and name O) (segid 3A4 and resid 121 and name O)	3.62	0.19	0.19
	assign (segid 3A4 and resid 120 and name O) (segid 3A4 and resid 122 and name C)	4.09	0.24	0.25
	assign (segid 3A4 and resid 120 and name O) (segid 3A4 and resid 122 and name CA)	4.22	0.19	0.18
	assign (segid 3A4 and resid 120 and name O) (segid 3A4 and resid 122 and name CB)	5.09	0.26	0.26
	assign (segid 3A4 and resid 120 and name O) (segid 3A4 and resid 122 and name N)	3.23	0.19	0.20
40	assign (segid 3A4 and resid 120 and name O) (segid 3A4 and resid 122 and name O)	4.95	0.38	0.39
	assign (segid 3A4 and resid 120 and name O) (segid 3A4 and resid 123 and name C)	4.17	0.51	0.51
	assign (segid 3A4 and resid 120 and name O) (segid 3A4 and resid 123 and name CA)	4.12	0.27	0.28
	assign (segid 3A4 and resid 120 and name O) (segid 3A4 and resid 123 and name CB)	4.30	0.28	0.28
	assign (segid 3A4 and resid 120 and name O) (segid 3A4 and resid 123 and name N)	3.48	0.18	0.17
45	assign (segid 3A4 and resid 120 and name O) (segid 3A4 and resid 123 and name O)	5.32	0.50	0.51
	assign (segid 3A4 and resid 120 and name O) (segid 3A4 and resid 124 and name C)	4.98	0.78	0.77
	assign (segid 3A4 and resid 120 and name O) (segid 3A4 and resid 124 and name CA)	4.14	0.81	0.81
	assign (segid 3A4 and resid 120 and name O) (segid 3A4 and resid 124 and name CB)	3.85	0.86	0.86
	assign (segid 3A4 and resid 120 and name O) (segid 3A4 and resid 124 and name N)	3.33	0.69	0.70
50	assign (segid 3A4 and resid 120 and name O) (segid 3A4 and resid 125 and name CA)	6.07	0.57	0.56
	assign (segid 3A4 and resid 120 and name O) (segid 3A4 and resid 125 and name CB)	6.07	0.49	0.48
	assign (segid 3A4 and resid 120 and name O) (segid 3A4 and resid 125 and name N)	4.86	0.61	0.62
	assign (segid 3A4 and resid 120 and name O) (segid 3A4 and resid 438 and name C)	6.10	0.47	0.47
	assign (segid 3A4 and resid 120 and name O) (segid 3A4 and resid 438 and name O)	5.09	0.40	0.41
55	assign (segid 3A4 and resid 120 and name O) (segid 3A4 and resid 439 and name C)	7.24	0.22	0.21
	assign (segid 3A4 and resid 120 and name O) (segid 3A4 and resid 439 and name CA)	6.57	0.19	0.20
	assign (segid 3A4 and resid 120 and name O) (segid 3A4 and resid 439 and name N)	6.77	0.38	0.39
	assign (segid 3A4 and resid 120 and name O) (segid 3A4 and resid 440 and name N)	6.83	0.23	0.24
	assign (segid 3A4 and resid 120 and name O) (segid 3A4 and resid 440 and name O)	7.61	0.18	0.18
60	assign (segid 3A4 and resid 121 and name C) (segid 3A4 and resid 121 and name CB)	2.53	0.02	0.01
	assign (segid 3A4 and resid 121 and name C) (segid 3A4 and resid 121 and name O)	1.23	0.00	0.00
	assign (segid 3A4 and resid 121 and name C) (segid 3A4 and resid 122 and name C)	3.03	0.05	0.05
	assign (segid 3A4 and resid 121 and name C) (segid 3A4 and resid 122 and name CA)	2.42	0.03	0.02
	assign (segid 3A4 and resid 121 and name C) (segid 3A4 and resid 122 and name CB)	3.69	0.04	0.05
65	assign (segid 3A4 and resid 121 and name C) (segid 3A4 and resid 122 and name N)	1.32	0.01	0.01
	assign (segid 3A4 and resid 121 and name C) (segid 3A4 and resid 122 and name O)	3.74	0.13	0.12
	assign (segid 3A4 and resid 121 and name C) (segid 3A4 and resid 123 and name C)	4.76	0.19	0.19
	assign (segid 3A4 and resid 121 and name C) (segid 3A4 and resid 123 and name CA)	4.63	0.20	0.20
	assign (segid 3A4 and resid 121 and name C) (segid 3A4 and resid 123 and name CB)	5.53	0.28	0.29
70	assign (segid 3A4 and resid 121 and name C) (segid 3A4 and resid 123 and name N)	3.44	0.21	0.20
	assign (segid 3A4 and resid 121 and name C) (segid 3A4 and resid 123 and name O)	5.78	0.26	0.26
	assign (segid 3A4 and resid 121 and name C) (segid 3A4 and resid 124 and name C)	4.92	0.16	0.16
	assign (segid 3A4 and resid 121 and name C) (segid 3A4 and resid 124 and name CA)	4.91	0.18	0.18
	assign (segid 3A4 and resid 121 and name C) (segid 3A4 and resid 124 and name CB)	5.09	0.18	0.17
75	assign (segid 3A4 and resid 121 and name C) (segid 3A4 and resid 124 and name N)	4.17	0.15	0.15
	assign (segid 3A4 and resid 121 and name C) (segid 3A4 and resid 124 and name O)	6.03	0.18	0.18
	assign (segid 3A4 and resid 121 and name C) (segid 3A4 and resid 125 and name C)	5.21	0.40	0.40
	assign (segid 3A4 and resid 121 and name C) (segid 3A4 and resid 125 and name CA)	4.73	0.16	0.16
	assign (segid 3A4 and resid 121 and name C) (segid 3A4 and resid 125 and name CB)	4.42	0.21	0.21
80	assign (segid 3A4 and resid 121 and name C) (segid 3A4 and resid 125 and name N)	4.06	0.13	0.13
	assign (segid 3A4 and resid 121 and name C) (segid 3A4 and resid 125 and name O)	6.35	0.36	0.36
	assign (segid 3A4 and resid 121 and name C) (segid 3A4 and resid 126 and name CA)	5.65	0.89	0.89
	assign (segid 3A4 and resid 121 and name C) (segid 3A4 and resid 126 and name N)	4.67	0.71	0.71

	assign (segid 3A4 and resid 121 and name C)	(segid 3A4 and resid 127 and name N)	6.39	0.86	0.85
	assign (segid 3A4 and resid 121 and name C)	(segid 3A4 and resid 263 and name C)	7.52	0.20	0.20
	assign (segid 3A4 and resid 121 and name C)	(segid 3A4 and resid 263 and name O)	7.64	0.20	0.20
	assign (segid 3A4 and resid 121 and name C)	(segid 3A4 and resid 264 and name CA)	6.36	0.33	0.33
5	assign (segid 3A4 and resid 121 and name C)	(segid 3A4 and resid 264 and name N)	6.94	0.28	0.28
	assign (segid 3A4 and resid 121 and name C)	(segid 3A4 and resid 267 and name CB)	7.50	0.28	0.28
	assign (segid 3A4 and resid 121 and name C)	(segid 3A4 and resid 438 and name C)	6.01	0.69	0.69
	assign (segid 3A4 and resid 121 and name C)	(segid 3A4 and resid 438 and name O)	5.01	0.65	0.65
	assign (segid 3A4 and resid 121 and name CA)	(segid 3A4 and resid 121 and name C)	1.53	0.01	0.02
10	assign (segid 3A4 and resid 121 and name CA)	(segid 3A4 and resid 121 and name CB)	1.53	0.01	0.02
	assign (segid 3A4 and resid 121 and name CA)	(segid 3A4 and resid 121 and name O)	2.39	0.02	0.01
	assign (segid 3A4 and resid 121 and name CA)	(segid 3A4 and resid 122 and name C)	4.45	0.04	0.04
	assign (segid 3A4 and resid 121 and name CA)	(segid 3A4 and resid 122 and name CA)	3.82	0.04	0.05
	assign (segid 3A4 and resid 121 and name CA)	(segid 3A4 and resid 122 and name CB)	4.89	0.04	0.04
15	assign (segid 3A4 and resid 121 and name CA)	(segid 3A4 and resid 122 and name N)	2.46	0.05	0.05
	assign (segid 3A4 and resid 121 and name CA)	(segid 3A4 and resid 122 and name O)	5.20	0.15	0.14
	assign (segid 3A4 and resid 121 and name CA)	(segid 3A4 and resid 123 and name C)	5.70	0.17	0.16
	assign (segid 3A4 and resid 121 and name CA)	(segid 3A4 and resid 123 and name CA)	5.68	0.17	0.18
	assign (segid 3A4 and resid 121 and name CA)	(segid 3A4 and resid 123 and name CB)	6.33	0.30	0.31
20	assign (segid 3A4 and resid 121 and name CA)	(segid 3A4 and resid 123 and name N)	4.59	0.17	0.17
	assign (segid 3A4 and resid 121 and name CA)	(segid 3A4 and resid 123 and name O)	6.76	0.20	0.20
	assign (segid 3A4 and resid 121 and name CA)	(segid 3A4 and resid 124 and name C)	5.50	0.28	0.27
	assign (segid 3A4 and resid 121 and name CA)	(segid 3A4 and resid 124 and name CA)	5.37	0.27	0.27
	assign (segid 3A4 and resid 121 and name CA)	(segid 3A4 and resid 124 and name CB)	5.10	0.28	0.29
25	assign (segid 3A4 and resid 121 and name CA)	(segid 3A4 and resid 124 and name N)	4.84	0.19	0.20
	assign (segid 3A4 and resid 121 and name CA)	(segid 3A4 and resid 124 and name O)	6.51	0.33	0.34
	assign (segid 3A4 and resid 121 and name CA)	(segid 3A4 and resid 125 and name C)	6.26	0.46	0.46
	assign (segid 3A4 and resid 121 and name CA)	(segid 3A4 and resid 125 and name CA)	5.52	0.25	0.26
	assign (segid 3A4 and resid 121 and name CA)	(segid 3A4 and resid 125 and name CB)	4.97	0.30	0.30
30	assign (segid 3A4 and resid 121 and name CA)	(segid 3A4 and resid 125 and name N)	4.85	0.21	0.21
	assign (segid 3A4 and resid 121 and name CA)	(segid 3A4 and resid 126 and name CA)	6.93	0.92	0.93
	assign (segid 3A4 and resid 121 and name CA)	(segid 3A4 and resid 126 and name N)	5.86	0.77	0.77
	assign (segid 3A4 and resid 121 and name CA)	(segid 3A4 and resid 127 and name CA)	8.91	0.65	0.65
	assign (segid 3A4 and resid 121 and name CA)	(segid 3A4 and resid 127 and name CB)	8.78	0.51	0.51
35	assign (segid 3A4 and resid 121 and name CA)	(segid 3A4 and resid 128 and name CA)	10.40	0.34	0.35
	assign (segid 3A4 and resid 121 and name CA)	(segid 3A4 and resid 128 and name CB)	9.95	0.40	0.40
	assign (segid 3A4 and resid 121 and name CA)	(segid 3A4 and resid 129 and name CA)	11.47	0.67	0.66
	assign (segid 3A4 and resid 121 and name CA)	(segid 3A4 and resid 129 and name CB)	10.83	0.75	0.74
	assign (segid 3A4 and resid 121 and name CA)	(segid 3A4 and resid 130 and name CA)	13.55	0.51	0.51
40	assign (segid 3A4 and resid 121 and name CA)	(segid 3A4 and resid 130 and name CB)	13.19	0.52	0.51
	assign (segid 3A4 and resid 121 and name CA)	(segid 3A4 and resid 131 and name CA)	14.88	0.56	0.56
	assign (segid 3A4 and resid 121 and name CA)	(segid 3A4 and resid 131 and name CB)	14.33	0.56	0.57
	assign (segid 3A4 and resid 121 and name CA)	(segid 3A4 and resid 132 and name CA)	16.09	0.52	0.52
	assign (segid 3A4 and resid 121 and name CA)	(segid 3A4 and resid 132 and name CB)	15.45	0.51	0.52
45	assign (segid 3A4 and resid 121 and name CA)	(segid 3A4 and resid 133 and name CA)	17.81	0.64	0.64
	assign (segid 3A4 and resid 121 and name CA)	(segid 3A4 and resid 133 and name CB)	17.32	0.73	0.73
	assign (segid 3A4 and resid 121 and name CA)	(segid 3A4 and resid 150 and name CA)	17.93	1.16	1.15
	assign (segid 3A4 and resid 121 and name CA)	(segid 3A4 and resid 255 and name CA)	18.36	0.54	0.53
	assign (segid 3A4 and resid 121 and name CA)	(segid 3A4 and resid 256 and name CA)	15.32	0.47	0.47
50	assign (segid 3A4 and resid 121 and name CA)	(segid 3A4 and resid 257 and name CA)	14.24	0.73	0.73
	assign (segid 3A4 and resid 121 and name CA)	(segid 3A4 and resid 258 and name CA)	15.10	0.43	0.42
	assign (segid 3A4 and resid 121 and name CA)	(segid 3A4 and resid 258 and name CB)	16.53	0.40	0.40
	assign (segid 3A4 and resid 121 and name CA)	(segid 3A4 and resid 259 and name CA)	13.29	0.26	0.27
	assign (segid 3A4 and resid 121 and name CA)	(segid 3A4 and resid 259 and name CB)	13.76	0.21	0.21
55	assign (segid 3A4 and resid 121 and name CA)	(segid 3A4 and resid 260 and name CA)	9.93	0.39	0.39
	assign (segid 3A4 and resid 121 and name CA)	(segid 3A4 and resid 260 and name CB)	9.91	0.57	0.57
	assign (segid 3A4 and resid 121 and name CA)	(segid 3A4 and resid 261 and name CA)	10.60	0.57	0.56
	assign (segid 3A4 and resid 121 and name CA)	(segid 3A4 and resid 262 and name CA)	11.90	0.41	0.41
	assign (segid 3A4 and resid 121 and name CA)	(segid 3A4 and resid 262 and name CB)	13.03	0.37	0.37
60	assign (segid 3A4 and resid 121 and name CA)	(segid 3A4 and resid 263 and name CA)	9.10	0.23	0.22
	assign (segid 3A4 and resid 121 and name CA)	(segid 3A4 and resid 263 and name CB)	8.62	0.16	0.15
	assign (segid 3A4 and resid 121 and name CA)	(segid 3A4 and resid 264 and name CA)	6.92	0.39	0.39
	assign (segid 3A4 and resid 121 and name CA)	(segid 3A4 and resid 265 and name CA)	10.34	0.42	0.42
	assign (segid 3A4 and resid 121 and name CA)	(segid 3A4 and resid 266 and name CA)	11.11	0.26	0.26
65	assign (segid 3A4 and resid 121 and name CA)	(segid 3A4 and resid 267 and name CA)	8.55	0.30	0.31
	assign (segid 3A4 and resid 121 and name CA)	(segid 3A4 and resid 267 and name CB)	7.10	0.28	0.28
	assign (segid 3A4 and resid 121 and name CA)	(segid 3A4 and resid 268 and name CA)	9.75	0.42	0.42
	assign (segid 3A4 and resid 121 and name CA)	(segid 3A4 and resid 268 and name CB)	9.91	0.43	0.42
	assign (segid 3A4 and resid 121 and name CA)	(segid 3A4 and resid 269 and name CA)	13.18	0.40	0.39
70	assign (segid 3A4 and resid 121 and name CA)	(segid 3A4 and resid 270 and name CA)	13.17	0.49	0.48
	assign (segid 3A4 and resid 121 and name CA)	(segid 3A4 and resid 270 and name CB)	12.60	0.45	0.45
	assign (segid 3A4 and resid 121 and name CA)	(segid 3A4 and resid 271 and name CA)	12.07	0.64	0.63
	assign (segid 3A4 and resid 121 and name CA)	(segid 3A4 and resid 271 and name CB)	10.84	0.65	0.65
	assign (segid 3A4 and resid 121 and name CA)	(segid 3A4 and resid 272 and name CA)	14.84	0.56	0.56
75	assign (segid 3A4 and resid 121 and name CA)	(segid 3A4 and resid 272 and name CB)	14.91	0.55	0.54
	assign (segid 3A4 and resid 121 and name CA)	(segid 3A4 and resid 273 and name CA)	17.28	0.55	0.56
	assign (segid 3A4 and resid 121 and name CA)	(segid 3A4 and resid 273 and name CB)	17.67	0.62	0.61
	assign (segid 3A4 and resid 121 and name CA)	(segid 3A4 and resid 274 and name CA)	17.68	0.51	0.51
	assign (segid 3A4 and resid 121 and name CA)	(segid 3A4 and resid 274 and name CB)	18.17	0.68	0.67
80	assign (segid 3A4 and resid 121 and name CA)	(segid 3A4 and resid 276 and name CA)	19.10	0.49	0.50
	assign (segid 3A4 and resid 121 and name CA)	(segid 3A4 and resid 276 and name CB)	18.44	0.53	0.53
	assign (segid 3A4 and resid 121 and name CA)	(segid 3A4 and resid 277 and name CA)	16.63	0.37	0.37
	assign (segid 3A4 and resid 121 and name CA)	(segid 3A4 and resid 277 and name CB)	15.70	0.33	0.33

	assign (segid 3A4 and resid 121 and name CA) (segid 3A4 and resid 280 and name CA)	19.21	0.44	0.44
	assign (segid 3A4 and resid 121 and name CA) (segid 3A4 and resid 280 and name CB)	17.84	0.44	0.44
	assign (segid 3A4 and resid 121 and name CA) (segid 3A4 and resid 281 and name CB)	18.73	0.54	0.54
	assign (segid 3A4 and resid 121 and name CA) (segid 3A4 and resid 308 and name CB)	17.96	0.97	0.97
5	assign (segid 3A4 and resid 121 and name CA) (segid 3A4 and resid 309 and name CA)	17.46	0.77	0.78
	assign (segid 3A4 and resid 121 and name CA) (segid 3A4 and resid 309 and name CB)	17.61	0.76	0.76
	assign (segid 3A4 and resid 121 and name CA) (segid 3A4 and resid 312 and name CA)	16.68	0.91	0.90
	assign (segid 3A4 and resid 121 and name CA) (segid 3A4 and resid 312 and name CB)	15.46	0.87	0.86
	assign (segid 3A4 and resid 121 and name CA) (segid 3A4 and resid 313 and name CA)	18.18	0.73	0.72
10	assign (segid 3A4 and resid 121 and name CA) (segid 3A4 and resid 313 and name CB)	18.81	0.67	0.66
	assign (segid 3A4 and resid 121 and name CA) (segid 3A4 and resid 316 and name CA)	17.06	0.90	0.89
	assign (segid 3A4 and resid 121 and name CA) (segid 3A4 and resid 318 and name CA)	17.24	0.78	0.78
	assign (segid 3A4 and resid 121 and name CA) (segid 3A4 and resid 318 and name CB)	16.18	0.85	0.84
	assign (segid 3A4 and resid 121 and name CA) (segid 3A4 and resid 397 and name CA)	18.17	0.34	0.34
	assign (segid 3A4 and resid 121 and name CA) (segid 3A4 and resid 397 and name CB)	18.43	0.42	0.41
15	assign (segid 3A4 and resid 121 and name CA) (segid 3A4 and resid 398 and name CA)	19.06	0.41	0.41
	assign (segid 3A4 and resid 121 and name CA) (segid 3A4 and resid 399 and name CA)	19.23	0.27	0.27
	assign (segid 3A4 and resid 121 and name CA) (segid 3A4 and resid 400 and name CA)	15.82	0.37	0.37
	assign (segid 3A4 and resid 121 and name CA) (segid 3A4 and resid 400 and name CB)	15.45	0.41	0.42
20	assign (segid 3A4 and resid 121 and name CA) (segid 3A4 and resid 401 and name CA)	14.35	0.33	0.32
	assign (segid 3A4 and resid 121 and name CA) (segid 3A4 and resid 402 and name CA)	16.67	0.37	0.36
	assign (segid 3A4 and resid 121 and name CA) (segid 3A4 and resid 402 and name CB)	18.17	0.36	0.37
	assign (segid 3A4 and resid 121 and name CA) (segid 3A4 and resid 403 and name CA)	16.16	0.46	0.46
	assign (segid 3A4 and resid 121 and name CA) (segid 3A4 and resid 403 and name CB)	16.60	0.56	0.55
25	assign (segid 3A4 and resid 121 and name CA) (segid 3A4 and resid 404 and name CA)	12.43	0.46	0.46
	assign (segid 3A4 and resid 121 and name CA) (segid 3A4 and resid 404 and name CB)	11.51	0.41	0.41
	assign (segid 3A4 and resid 121 and name CA) (segid 3A4 and resid 405 and name CA)	12.71	0.53	0.53
	assign (segid 3A4 and resid 121 and name CA) (segid 3A4 and resid 405 and name CB)	13.25	0.54	0.53
	assign (segid 3A4 and resid 121 and name CA) (segid 3A4 and resid 406 and name CA)	15.79	0.54	0.53
30	assign (segid 3A4 and resid 121 and name CA) (segid 3A4 and resid 407 and name CA)	14.49	0.62	0.61
	assign (segid 3A4 and resid 121 and name CA) (segid 3A4 and resid 407 and name CB)	14.37	0.68	0.69
	assign (segid 3A4 and resid 121 and name CA) (segid 3A4 and resid 408 and name CA)	11.30	0.64	0.65
	assign (segid 3A4 and resid 121 and name CA) (segid 3A4 and resid 408 and name CB)	10.12	0.54	0.53
	assign (segid 3A4 and resid 121 and name CA) (segid 3A4 and resid 409 and name CA)	13.51	0.61	0.60
35	assign (segid 3A4 and resid 121 and name CA) (segid 3A4 and resid 409 and name CB)	14.09	0.61	0.62
	assign (segid 3A4 and resid 121 and name CA) (segid 3A4 and resid 410 and name CA)	16.30	0.58	0.58
	assign (segid 3A4 and resid 121 and name CA) (segid 3A4 and resid 411 and name CA)	14.65	0.70	0.70
	assign (segid 3A4 and resid 121 and name CA) (segid 3A4 and resid 411 and name CB)	13.91	0.86	0.86
	assign (segid 3A4 and resid 121 and name CA) (segid 3A4 and resid 412 and name CA)	12.91	0.49	0.48
40	assign (segid 3A4 and resid 121 and name CA) (segid 3A4 and resid 413 and name CA)	13.66	0.81	0.82
	assign (segid 3A4 and resid 121 and name CA) (segid 3A4 and resid 414 and name CA)	10.94	0.43	0.42
	assign (segid 3A4 and resid 121 and name CA) (segid 3A4 and resid 415 and name CA)	11.15	0.78	0.77
	assign (segid 3A4 and resid 121 and name CA) (segid 3A4 and resid 415 and name CB)	12.19	0.81	0.82
	assign (segid 3A4 and resid 121 and name CA) (segid 3A4 and resid 416 and name CA)	10.54	0.82	0.83
45	assign (segid 3A4 and resid 121 and name CA) (segid 3A4 and resid 417 and name CA)	12.25	1.40	1.40
	assign (segid 3A4 and resid 121 and name CA) (segid 3A4 and resid 423 and name CA)	13.91	1.37	1.38
	assign (segid 3A4 and resid 121 and name CA) (segid 3A4 and resid 424 and name CA)	12.93	1.28	1.29
	assign (segid 3A4 and resid 121 and name CA) (segid 3A4 and resid 425 and name CA)	13.28	1.60	1.60
	assign (segid 3A4 and resid 121 and name CA) (segid 3A4 and resid 426 and name CA)	14.18	0.98	0.98
50	assign (segid 3A4 and resid 121 and name CA) (segid 3A4 and resid 427 and name CA)	15.22	1.16	1.16
	assign (segid 3A4 and resid 121 and name CA) (segid 3A4 and resid 428 and name CA)	17.71	1.78	1.78
	assign (segid 3A4 and resid 121 and name CA) (segid 3A4 and resid 433 and name CA)	16.14	0.87	0.87
	assign (segid 3A4 and resid 121 and name CA) (segid 3A4 and resid 434 and name CA)	12.67	0.97	0.98
	assign (segid 3A4 and resid 121 and name CA) (segid 3A4 and resid 435 and name CA)	10.23	0.77	0.76
55	assign (segid 3A4 and resid 121 and name CA) (segid 3A4 and resid 436 and name CA)	10.04	0.79	0.79
	assign (segid 3A4 and resid 121 and name CA) (segid 3A4 and resid 437 and name CA)	7.73	0.72	0.72
	assign (segid 3A4 and resid 121 and name CA) (segid 3A4 and resid 438 and name C)	5.33	0.70	0.69
	assign (segid 3A4 and resid 121 and name CA) (segid 3A4 and resid 438 and name CA)	6.00	0.84	0.83
	assign (segid 3A4 and resid 121 and name CA) (segid 3A4 and resid 438 and name O)	4.23	0.71	0.71
60	assign (segid 3A4 and resid 121 and name CA) (segid 3A4 and resid 439 and name C)	6.52	0.36	0.36
	assign (segid 3A4 and resid 121 and name CA) (segid 3A4 and resid 439 and name CA)	6.27	0.38	0.39
	assign (segid 3A4 and resid 121 and name CA) (segid 3A4 and resid 439 and name N)	6.25	0.54	0.55
	assign (segid 3A4 and resid 121 and name CA) (segid 3A4 and resid 440 and name C)	7.45	0.20	0.19
	assign (segid 3A4 and resid 121 and name CA) (segid 3A4 and resid 440 and name CA)	6.75	0.37	0.37
65	assign (segid 3A4 and resid 121 and name CA) (segid 3A4 and resid 440 and name N)	6.08	0.34	0.35
	assign (segid 3A4 and resid 121 and name CA) (segid 3A4 and resid 440 and name O)	7.23	0.14	0.13
	assign (segid 3A4 and resid 121 and name CA) (segid 3A4 and resid 440 and name C)	5.51	0.06	0.06
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 122 and name CA)	4.59	0.05	0.05
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 122 and name CB)	5.51	0.12	0.11
70	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 122 and name N)	3.30	0.06	0.06
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 122 and name O)	6.19	0.10	0.10
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 123 and name C)	7.07	0.21	0.22
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 123 and name CA)	7.04	0.19	0.19
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 123 and name CB)	7.75	0.27	0.27
75	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 123 and name N)	5.86	0.17	0.16
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 124 and name C)	6.59	0.25	0.26
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 124 and name CA)	6.68	0.24	0.24
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 124 and name CB)	6.36	0.26	0.26
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 124 and name N)	6.25	0.17	0.17
80	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 125 and name CA)	6.19	0.33	0.33
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 125 and name CB)	5.36	0.39	0.40
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 125 and name N)	5.81	0.26	0.26
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 126 and name CA)	7.38	1.11	1.10

	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 127 and name CA)	9.76	0.73	0.73
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 127 and name CB)	9.77	0.57	0.58
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 128 and name CA)	11.19	0.24	0.25
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 128 and name CB)	10.75	0.39	0.39
5	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 129 and name CA)	11.91	0.63	0.63
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 129 and name CB)	11.13	0.74	0.74
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 130 and name CA)	13.99	0.66	0.67
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 130 and name CB)	13.62	0.75	0.75
10	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 131 and name CA)	15.56	0.59	0.60
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 131 and name CB)	15.11	0.58	0.58
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 132 and name CA)	16.71	0.39	0.38
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 132 and name CB)	16.05	0.32	0.31
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 133 and name CA)	18.24	0.63	0.63
15	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 133 and name CB)	17.67	0.75	0.76
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 255 and name CA)	18.53	0.54	0.55
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 256 and name CA)	15.68	0.45	0.45
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 257 and name CA)	14.48	0.73	0.74
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 258 and name CA)	14.96	0.44	0.45
20	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 258 and name CB)	16.37	0.42	0.42
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 259 and name CA)	13.09	0.28	0.28
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 259 and name CB)	13.64	0.24	0.23
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 260 and name CA)	9.93	0.40	0.41
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 260 and name CB)	10.13	0.57	0.56
25	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 261 and name CA)	10.28	0.60	0.60
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 262 and name CA)	11.20	0.45	0.45
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 262 and name CB)	12.35	0.39	0.40
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 263 and name C)	7.19	0.31	0.31
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 263 and name CA)	8.33	0.25	0.25
30	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 263 and name CB)	8.03	0.18	0.19
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 263 and name O)	6.90	0.33	0.33
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 264 and name C)	6.91	0.47	0.46
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 264 and name CA)	6.06	0.46	0.45
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 264 and name N)	6.85	0.39	0.40
35	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 264 and name O)	6.60	0.47	0.46
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 265 and name CA)	9.26	0.48	0.49
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 266 and name CA)	9.82	0.31	0.31
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 267 and name CA)	7.11	0.31	0.31
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 267 and name CB)	5.67	0.29	0.28
40	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 268 and name CA)	8.36	0.47	0.47
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 268 and name CB)	8.64	0.50	0.49
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 269 and name CA)	11.73	0.42	0.43
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 270 and name CA)	11.66	0.48	0.48
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 270 and name CB)	11.12	0.44	0.43
45	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 271 and name CA)	10.63	0.62	0.62
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 271 and name CB)	9.43	0.64	0.65
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 272 and name CA)	13.43	0.57	0.56
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 272 and name CB)	13.51	0.57	0.57
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 273 and name CA)	15.80	0.55	0.55
50	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 273 and name CB)	16.17	0.61	0.62
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 274 and name CA)	16.23	0.48	0.48
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 274 and name CB)	16.75	0.64	0.64
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 276 and name CA)	17.62	0.47	0.47
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 276 and name CB)	16.95	0.52	0.51
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 277 and name CA)	15.20	0.33	0.32
55	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 277 and name CB)	14.27	0.29	0.30
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 278 and name CA)	18.37	0.26	0.25
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 278 and name CB)	19.34	0.32	0.32
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 280 and name CA)	17.88	0.38	0.39
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 280 and name CB)	16.51	0.40	0.39
60	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 281 and name CA)	17.90	0.57	0.57
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 281 and name CB)	17.51	0.51	0.50
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 305 and name CA)	18.22	0.80	0.79
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 305 and name CB)	17.79	0.78	0.78
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 308 and name CA)	17.50	0.91	0.91
65	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 308 and name CB)	16.65	0.92	0.93
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 309 and name CA)	16.35	0.73	0.73
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 309 and name CB)	16.57	0.70	0.70
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 312 and name CA)	15.48	0.90	0.90
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 312 and name CB)	14.26	0.85	0.85
70	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 313 and name CA)	17.19	0.74	0.73
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 313 and name CB)	17.87	0.67	0.67
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 315 and name CA)	18.40	0.91	0.92
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 315 and name CB)	17.74	0.93	0.93
75	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 316 and name CA)	16.08	0.94	0.94
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 317 and name CA)	18.33	0.80	0.80
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 318 and name CA)	16.69	0.76	0.76
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 318 and name CB)	15.66	0.83	0.83
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 363 and name CB)	17.78	1.04	1.03
80	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 397 and name CA)	17.80	0.27	0.27
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 397 and name CB)	18.03	0.36	0.36
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 398 and name CA)	18.43	0.31	0.30
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 399 and name CA)	18.73	0.26	0.26
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 400 and name CA)	15.47	0.43	0.43

	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 400 and name CB)	15.20	0.49	0.50
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 401 and name CA)	13.69	0.19	0.18
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 402 and name CA)	15.87	0.28	0.27
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 402 and name CB)	17.38	0.28	0.27
5	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 403 and name CA)	15.60	0.48	0.47
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 403 and name CB)	16.16	0.57	0.57
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 404 and name CA)	11.88	0.52	0.53
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 404 and name CB)	11.00	0.50	0.50
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 405 and name CA)	11.78	0.54	0.53
10	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 405 and name CB)	12.22	0.51	0.51
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 406 and name CA)	14.91	0.61	0.60
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 407 and name CA)	13.87	0.71	0.70
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 407 and name CB)	13.89	0.74	0.74
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 408 and name CA)	10.56	0.76	0.77
15	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 408 and name CB)	9.30	0.67	0.67
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 409 and name CA)	12.48	0.71	0.72
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 409 and name CB)	12.97	0.72	0.72
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 410 and name CA)	15.47	0.69	0.68
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 411 and name CA)	14.07	0.79	0.79
20	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 411 and name CB)	13.44	0.95	0.96
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 412 and name CA)	12.15	0.58	0.59
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 413 and name CA)	12.67	0.81	0.82
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 414 and name CA)	9.86	0.46	0.45
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 415 and name CA)	10.10	0.82	0.82
25	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 415 and name CB)	11.20	0.86	0.86
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 416 and name CA)	9.64	0.93	0.93
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 417 and name CA)	11.70	1.43	1.42
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 423 and name CA)	13.31	1.43	1.44
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 424 and name CA)	12.28	1.22	1.21
30	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 425 and name CA)	12.81	1.55	1.56
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 426 and name CA)	13.77	0.97	0.97
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 427 and name CA)	15.00	1.28	1.28
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 428 and name CA)	17.60	1.83	1.83
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 433 and name CA)	15.81	0.87	0.86
35	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 434 and name CA)	12.35	0.97	0.97
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 435 and name CA)	9.85	0.81	0.80
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 436 and name CA)	10.15	0.69	0.68
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 437 and name CA)	7.95	0.63	0.63
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 438 and name C)	5.08	0.73	0.72
40	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 438 and name CA)	5.65	0.87	0.86
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 438 and name N)	6.06	0.74	0.74
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 438 and name O)	4.08	0.76	0.76
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 439 and name C)	6.13	0.40	0.40
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 439 and name CA)	6.16	0.43	0.43
45	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 439 and name N)	6.04	0.58	0.58
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 439 and name O)	6.82	0.44	0.44
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 440 and name C)	7.04	0.24	0.24
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 440 and name CA)	6.17	0.39	0.40
	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 440 and name N)	5.72	0.35	0.36
50	assign (segid 3A4 and resid 121 and name CB) (segid 3A4 and resid 440 and name O)	7.06	0.20	0.20
	assign (segid 3A4 and resid 121 and name N) (segid 3A4 and resid 121 and name C)	2.49	0.01	0.01
	assign (segid 3A4 and resid 121 and name N) (segid 3A4 and resid 121 and name CA)	1.45	0.00	0.01
	assign (segid 3A4 and resid 121 and name N) (segid 3A4 and resid 121 and name CB)	2.44	0.05	0.04
	assign (segid 3A4 and resid 121 and name N) (segid 3A4 and resid 121 and name O)	3.55	0.05	0.06
55	assign (segid 3A4 and resid 121 and name N) (segid 3A4 and resid 122 and name C)	4.86	0.10	0.09
	assign (segid 3A4 and resid 121 and name N) (segid 3A4 and resid 122 and name CA)	4.26	0.10	0.11
	assign (segid 3A4 and resid 121 and name N) (segid 3A4 and resid 122 and name CB)	5.02	0.12	0.12
	assign (segid 3A4 and resid 121 and name N) (segid 3A4 and resid 122 and name N)	2.84	0.12	0.12
	assign (segid 3A4 and resid 121 and name N) (segid 3A4 and resid 122 and name O)	5.81	0.19	0.19
60	assign (segid 3A4 and resid 121 and name N) (segid 3A4 and resid 123 and name C)	5.94	0.24	0.24
	assign (segid 3A4 and resid 121 and name N) (segid 3A4 and resid 123 and name CA)	5.75	0.17	0.17
	assign (segid 3A4 and resid 121 and name N) (segid 3A4 and resid 123 and name CB)	6.09	0.29	0.29
	assign (segid 3A4 and resid 121 and name N) (segid 3A4 and resid 123 and name N)	4.68	0.12	0.12
	assign (segid 3A4 and resid 121 and name N) (segid 3A4 and resid 123 and name O)	7.09	0.18	0.17
65	assign (segid 3A4 and resid 121 and name N) (segid 3A4 and resid 124 and name C)	6.26	0.44	0.45
	assign (segid 3A4 and resid 121 and name N) (segid 3A4 and resid 124 and name CA)	5.82	0.48	0.48
	assign (segid 3A4 and resid 121 and name N) (segid 3A4 and resid 124 and name CB)	5.40	0.54	0.55
	assign (segid 3A4 and resid 121 and name N) (segid 3A4 and resid 124 and name N)	5.13	0.39	0.40
	assign (segid 3A4 and resid 121 and name N) (segid 3A4 and resid 125 and name CA)	6.67	0.28	0.29
70	assign (segid 3A4 and resid 121 and name N) (segid 3A4 and resid 125 and name CB)	6.23	0.32	0.31
	assign (segid 3A4 and resid 121 and name N) (segid 3A4 and resid 125 and name N)	5.81	0.30	0.30
	assign (segid 3A4 and resid 121 and name N) (segid 3A4 and resid 438 and name C)	4.38	0.59	0.60
	assign (segid 3A4 and resid 121 and name N) (segid 3A4 and resid 438 and name CA)	5.27	0.71	0.71
	assign (segid 3A4 and resid 121 and name N) (segid 3A4 and resid 438 and name N)	5.34	0.71	0.71
75	assign (segid 3A4 and resid 121 and name N) (segid 3A4 and resid 438 and name O)	3.28	0.61	0.60
	assign (segid 3A4 and resid 121 and name N) (segid 3A4 and resid 439 and name C)	5.53	0.30	0.31
	assign (segid 3A4 and resid 121 and name N) (segid 3A4 and resid 439 and name CA)	5.09	0.32	0.31
	assign (segid 3A4 and resid 121 and name N) (segid 3A4 and resid 439 and name N)	5.17	0.47	0.47
	assign (segid 3A4 and resid 121 and name N) (segid 3A4 and resid 439 and name O)	6.52	0.32	0.32
80	assign (segid 3A4 and resid 121 and name N) (segid 3A4 and resid 440 and name C)	6.76	0.19	0.19
	assign (segid 3A4 and resid 121 and name N) (segid 3A4 and resid 440 and name CA)	6.08	0.33	0.34
	assign (segid 3A4 and resid 121 and name N) (segid 3A4 and resid 440 and name N)	5.18	0.31	0.32
	assign (segid 3A4 and resid 121 and name N) (segid 3A4 and resid 440 and name O)	6.43	0.11	0.11

	assign (segid 3A4 and resid 121 and name O)	(segid 3A4 and resid 121 and name CB)	3.21	0.09	0.08
	assign (segid 3A4 and resid 121 and name O)	(segid 3A4 and resid 122 and name C)	2.97	0.10	0.10
	assign (segid 3A4 and resid 121 and name O)	(segid 3A4 and resid 122 and name CA)	2.73	0.05	0.05
	assign (segid 3A4 and resid 121 and name O)	(segid 3A4 and resid 122 and name CB)	4.21	0.07	0.07
	assign (segid 3A4 and resid 121 and name O)	(segid 3A4 and resid 122 and name N)	2.23	0.03	0.03
5	assign (segid 3A4 and resid 121 and name O)	(segid 3A4 and resid 122 and name O)	3.28	0.13	0.13
	assign (segid 3A4 and resid 121 and name O)	(segid 3A4 and resid 123 and name C)	4.41	0.38	0.37
	assign (segid 3A4 and resid 121 and name O)	(segid 3A4 and resid 123 and name CA)	4.56	0.36	0.35
	assign (segid 3A4 and resid 121 and name O)	(segid 3A4 and resid 123 and name CB)	5.67	0.44	0.44
	assign (segid 3A4 and resid 121 and name O)	(segid 3A4 and resid 123 and name N)	3.58	0.33	0.33
10	assign (segid 3A4 and resid 121 and name O)	(segid 3A4 and resid 123 and name O)	5.27	0.44	0.44
	assign (segid 3A4 and resid 121 and name O)	(segid 3A4 and resid 124 and name C)	4.08	0.11	0.12
	assign (segid 3A4 and resid 121 and name O)	(segid 3A4 and resid 124 and name CA)	4.37	0.21	0.21
	assign (segid 3A4 and resid 121 and name O)	(segid 3A4 and resid 124 and name CB)	4.73	0.24	0.25
	assign (segid 3A4 and resid 121 and name O)	(segid 3A4 and resid 124 and name N)	3.83	0.26	0.25
15	assign (segid 3A4 and resid 121 and name O)	(segid 3A4 and resid 124 and name O)	5.14	0.06	0.05
	assign (segid 3A4 and resid 121 and name O)	(segid 3A4 and resid 125 and name C)	4.03	0.43	0.42
	assign (segid 3A4 and resid 121 and name O)	(segid 3A4 and resid 125 and name CA)	3.59	0.13	0.14
	assign (segid 3A4 and resid 121 and name O)	(segid 3A4 and resid 125 and name CB)	3.40	0.20	0.19
	assign (segid 3A4 and resid 121 and name O)	(segid 3A4 and resid 125 and name N)	3.06	0.11	0.11
20	assign (segid 3A4 and resid 121 and name O)	(segid 3A4 and resid 125 and name O)	5.18	0.38	0.38
	assign (segid 3A4 and resid 121 and name O)	(segid 3A4 and resid 126 and name C)	5.57	0.87	0.88
	assign (segid 3A4 and resid 121 and name O)	(segid 3A4 and resid 126 and name CA)	4.62	0.90	0.91
	assign (segid 3A4 and resid 121 and name O)	(segid 3A4 and resid 126 and name N)	3.53	0.76	0.76
25	assign (segid 3A4 and resid 121 and name O)	(segid 3A4 and resid 127 and name CB)	6.77	0.58	0.57
	assign (segid 3A4 and resid 121 and name O)	(segid 3A4 and resid 127 and name N)	5.43	0.79	0.79
	assign (segid 3A4 and resid 121 and name O)	(segid 3A4 and resid 260 and name O)	6.94	0.39	0.40
	assign (segid 3A4 and resid 121 and name O)	(segid 3A4 and resid 263 and name C)	7.21	0.17	0.17
	assign (segid 3A4 and resid 121 and name O)	(segid 3A4 and resid 263 and name CB)	7.18	0.14	0.15
30	assign (segid 3A4 and resid 121 and name O)	(segid 3A4 and resid 263 and name O)	7.41	0.17	0.17
	assign (segid 3A4 and resid 121 and name O)	(segid 3A4 and resid 264 and name CA)	6.41	0.31	0.30
	assign (segid 3A4 and resid 121 and name O)	(segid 3A4 and resid 264 and name N)	6.72	0.27	0.27
	assign (segid 3A4 and resid 121 and name O)	(segid 3A4 and resid 438 and name O)	6.20	0.66	0.65
	assign (segid 3A4 and resid 121 and name O)	(segid 3A4 and resid 122 and name CB)	2.54	0.03	0.02
35	assign (segid 3A4 and resid 122 and name C)	(segid 3A4 and resid 122 and name O)	1.24	0.01	0.01
	assign (segid 3A4 and resid 122 and name C)	(segid 3A4 and resid 123 and name C)	3.14	0.05	0.04
	assign (segid 3A4 and resid 122 and name C)	(segid 3A4 and resid 123 and name CA)	2.44	0.02	0.02
	assign (segid 3A4 and resid 122 and name C)	(segid 3A4 and resid 123 and name CB)	3.70	0.02	0.02
	assign (segid 3A4 and resid 122 and name C)	(segid 3A4 and resid 123 and name N)	1.33	0.00	0.01
40	assign (segid 3A4 and resid 122 and name C)	(segid 3A4 and resid 123 and name O)	3.96	0.18	0.17
	assign (segid 3A4 and resid 122 and name C)	(segid 3A4 and resid 124 and name C)	4.83	0.17	0.18
	assign (segid 3A4 and resid 122 and name C)	(segid 3A4 and resid 124 and name CA)	4.68	0.16	0.16
	assign (segid 3A4 and resid 122 and name C)	(segid 3A4 and resid 124 and name CB)	5.60	0.16	0.17
	assign (segid 3A4 and resid 122 and name C)	(segid 3A4 and resid 124 and name N)	3.48	0.18	0.17
	assign (segid 3A4 and resid 122 and name C)	(segid 3A4 and resid 124 and name O)	5.98	0.19	0.19
45	assign (segid 3A4 and resid 122 and name C)	(segid 3A4 and resid 125 and name C)	4.83	0.18	0.18
	assign (segid 3A4 and resid 122 and name C)	(segid 3A4 and resid 125 and name CA)	4.89	0.22	0.23
	assign (segid 3A4 and resid 122 and name C)	(segid 3A4 and resid 125 and name CB)	5.32	0.51	0.51
	assign (segid 3A4 and resid 122 and name C)	(segid 3A4 and resid 125 and name N)	4.06	0.19	0.19
	assign (segid 3A4 and resid 122 and name C)	(segid 3A4 and resid 125 and name O)	5.75	0.24	0.24
50	assign (segid 3A4 and resid 122 and name C)	(segid 3A4 and resid 126 and name C)	5.21	0.59	0.59
	assign (segid 3A4 and resid 122 and name C)	(segid 3A4 and resid 126 and name CA)	4.80	0.22	0.22
	assign (segid 3A4 and resid 122 and name C)	(segid 3A4 and resid 126 and name N)	4.18	0.15	0.16
	assign (segid 3A4 and resid 122 and name C)	(segid 3A4 and resid 126 and name O)	6.33	0.58	0.58
	assign (segid 3A4 and resid 122 and name C)	(segid 3A4 and resid 127 and name CA)	5.66	1.06	1.06
55	assign (segid 3A4 and resid 122 and name C)	(segid 3A4 and resid 127 and name CB)	5.36	1.29	1.28
	assign (segid 3A4 and resid 122 and name C)	(segid 3A4 and resid 127 and name N)	4.70	0.87	0.88
	assign (segid 3A4 and resid 122 and name C)	(segid 3A4 and resid 260 and name CB)	6.94	0.53	0.53
	assign (segid 3A4 and resid 122 and name C)	(segid 3A4 and resid 260 and name O)	6.95	0.41	0.42
60	assign (segid 3A4 and resid 122 and name C)	(segid 3A4 and resid 264 and name CA)	7.41	0.29	0.30
	assign (segid 3A4 and resid 122 and name CA)	(segid 3A4 and resid 122 and name C)	1.52	0.01	0.01
	assign (segid 3A4 and resid 122 and name CA)	(segid 3A4 and resid 122 and name CB)	1.54	0.01	0.02
	assign (segid 3A4 and resid 122 and name CA)	(segid 3A4 and resid 122 and name O)	2.41	0.01	0.01
	assign (segid 3A4 and resid 122 and name CA)	(segid 3A4 and resid 123 and name C)	4.53	0.05	0.04
65	assign (segid 3A4 and resid 122 and name CA)	(segid 3A4 and resid 123 and name CA)	3.81	0.02	0.02
	assign (segid 3A4 and resid 122 and name CA)	(segid 3A4 and resid 123 and name CB)	4.85	0.03	0.02
	assign (segid 3A4 and resid 122 and name CA)	(segid 3A4 and resid 123 and name N)	2.43	0.01	0.02
	assign (segid 3A4 and resid 122 and name CA)	(segid 3A4 and resid 123 and name O)	5.42	0.18	0.18
	assign (segid 3A4 and resid 122 and name CA)	(segid 3A4 and resid 124 and name C)	5.78	0.16	0.16
70	assign (segid 3A4 and resid 122 and name CA)	(segid 3A4 and resid 124 and name CA)	5.73	0.17	0.17
	assign (segid 3A4 and resid 122 and name CA)	(segid 3A4 and resid 124 and name CB)	6.40	0.18	0.19
	assign (segid 3A4 and resid 122 and name CA)	(segid 3A4 and resid 124 and name N)	4.61	0.18	0.18
	assign (segid 3A4 and resid 122 and name CA)	(segid 3A4 and resid 124 and name O)	6.93	0.17	0.17
	assign (segid 3A4 and resid 122 and name CA)	(segid 3A4 and resid 125 and name C)	5.41	0.23	0.22
75	assign (segid 3A4 and resid 122 and name CA)	(segid 3A4 and resid 125 and name CA)	5.47	0.21	0.21
	assign (segid 3A4 and resid 122 and name CA)	(segid 3A4 and resid 125 and name CB)	5.51	0.53	0.54
	assign (segid 3A4 and resid 122 and name CA)	(segid 3A4 and resid 125 and name N)	4.84	0.17	0.17
	assign (segid 3A4 and resid 122 and name CA)	(segid 3A4 and resid 125 and name O)	6.37	0.25	0.25
	assign (segid 3A4 and resid 122 and name CA)	(segid 3A4 and resid 126 and name C)	5.81	0.96	0.96
80	assign (segid 3A4 and resid 122 and name CA)	(segid 3A4 and resid 126 and name CA)	5.15	0.64	0.64
	assign (segid 3A4 and resid 122 and name CA)	(segid 3A4 and resid 126 and name N)	4.64	0.41	0.41
	assign (segid 3A4 and resid 122 and name CA)	(segid 3A4 and resid 127 and name CA)	6.65	1.27	1.27
	assign (segid 3A4 and resid 122 and name CA)	(segid 3A4 and resid 127 and name CB)	6.51	1.40	1.41

assign (segid 3A4 and resid 122 and name CA) (segid 3A4 and resid 127 and name N) 5.57 1.14 1.13
assign (segid 3A4 and resid 122 and name CA) (segid 3A4 and resid 128 and name CA) 9.07 0.78 0.78
assign (segid 3A4 and resid 122 and name CA) (segid 3A4 and resid 128 and name CB) 9.05 0.65 0.65
assign (segid 3A4 and resid 122 and name CA) (segid 3A4 and resid 129 and name CA) 10.22 0.56 0.57
5 assign (segid 3A4 and resid 122 and name CA) (segid 3A4 and resid 129 and name CB) 9.72 0.44 0.45
assign (segid 3A4 and resid 122 and name CA) (segid 3A4 and resid 130 and name CA) 11.58 0.50 0.49
assign (segid 3A4 and resid 122 and name CA) (segid 3A4 and resid 130 and name CB) 11.03 0.54 0.53
assign (segid 3A4 and resid 122 and name CA) (segid 3A4 and resid 131 and name CA) 12.87 0.97 0.98
assign (segid 3A4 and resid 122 and name CA) (segid 3A4 and resid 131 and name CB) 12.34 1.16 1.15
10 assign (segid 3A4 and resid 122 and name CA) (segid 3A4 and resid 132 and name CA) 14.62 0.76 0.75
assign (segid 3A4 and resid 122 and name CA) (segid 3A4 and resid 132 and name CB) 14.22 0.68 0.67
assign (segid 3A4 and resid 122 and name CA) (segid 3A4 and resid 133 and name CA) 16.19 0.62 0.61
assign (segid 3A4 and resid 122 and name CA) (segid 3A4 and resid 133 and name CB) 15.67 0.59 0.60
assign (segid 3A4 and resid 122 and name CA) (segid 3A4 and resid 134 and name CA) 17.35 0.58 0.59
15 assign (segid 3A4 and resid 122 and name CA) (segid 3A4 and resid 150 and name CA) 15.54 1.03 1.03
assign (segid 3A4 and resid 122 and name CA) (segid 3A4 and resid 151 and name CA) 15.71 1.56 1.56
assign (segid 3A4 and resid 122 and name CA) (segid 3A4 and resid 152 and name CA) 17.04 0.88 0.88
assign (segid 3A4 and resid 122 and name CA) (segid 3A4 and resid 153 and name CA) 15.48 1.31 1.32
20 assign (segid 3A4 and resid 122 and name CA) (segid 3A4 and resid 153 and name CB) 15.33 1.83 1.83
assign (segid 3A4 and resid 122 and name CA) (segid 3A4 and resid 154 and name CA) 13.76 1.41 1.40
assign (segid 3A4 and resid 122 and name CA) (segid 3A4 and resid 155 and name CA) 15.51 1.97 1.96
assign (segid 3A4 and resid 122 and name CA) (segid 3A4 and resid 156 and name CA) 16.59 1.03 1.04
assign (segid 3A4 and resid 122 and name CA) (segid 3A4 and resid 156 and name CB) 16.93 1.31 1.31
25 assign (segid 3A4 and resid 122 and name CA) (segid 3A4 and resid 157 and name CA) 14.83 1.26 1.27
assign (segid 3A4 and resid 122 and name CA) (segid 3A4 and resid 157 and name CB) 14.07 1.44 1.45
assign (segid 3A4 and resid 122 and name CA) (segid 3A4 and resid 160 and name CA) 17.94 1.36 1.36
30 assign (segid 3A4 and resid 122 and name CA) (segid 3A4 and resid 252 and name CA) 17.80 0.69 0.69
assign (segid 3A4 and resid 122 and name CA) (segid 3A4 and resid 252 and name CB) 18.26 0.76 0.75
assign (segid 3A4 and resid 122 and name CA) (segid 3A4 and resid 253 and name CA) 16.75 0.41 0.41
35 assign (segid 3A4 and resid 122 and name CA) (segid 3A4 and resid 254 and name CA) 17.24 0.53 0.54
assign (segid 3A4 and resid 122 and name CA) (segid 3A4 and resid 255 and name CA) 15.54 0.55 0.55
assign (segid 3A4 and resid 122 and name CA) (segid 3A4 and resid 256 and name CA) 12.32 0.48 0.47
assign (segid 3A4 and resid 122 and name CA) (segid 3A4 and resid 257 and name CA) 10.88 0.79 0.78
40 assign (segid 3A4 and resid 122 and name CA) (segid 3A4 and resid 258 and name CA) 12.22 0.49 0.49
assign (segid 3A4 and resid 122 and name CA) (segid 3A4 and resid 258 and name CB) 13.73 0.48 0.47
35 assign (segid 3A4 and resid 122 and name CA) (segid 3A4 and resid 259 and name CA) 11.06 0.34 0.35
assign (segid 3A4 and resid 122 and name CA) (segid 3A4 and resid 259 and name CB) 11.65 0.33 0.34
assign (segid 3A4 and resid 122 and name CA) (segid 3A4 and resid 260 and name C) 7.02 0.41 0.42
40 assign (segid 3A4 and resid 122 and name CA) (segid 3A4 and resid 260 and name CA) 7.37 0.38 0.38
assign (segid 3A4 and resid 122 and name CA) (segid 3A4 and resid 260 and name CB) 6.97 0.51 0.52
assign (segid 3A4 and resid 122 and name CA) (segid 3A4 and resid 260 and name O) 6.32 0.41 0.41
45 assign (segid 3A4 and resid 122 and name CA) (segid 3A4 and resid 261 and name CA) 7.99 0.57 0.57
assign (segid 3A4 and resid 122 and name CA) (segid 3A4 and resid 262 and name CA) 10.29 0.37 0.38
assign (segid 3A4 and resid 122 and name CA) (segid 3A4 and resid 262 and name CB) 11.44 0.36 0.36
50 assign (segid 3A4 and resid 122 and name CA) (segid 3A4 and resid 263 and name C) 7.60 0.19 0.19
assign (segid 3A4 and resid 122 and name CA) (segid 3A4 and resid 263 and name CA) 8.42 0.22 0.22
assign (segid 3A4 and resid 122 and name CA) (segid 3A4 and resid 263 and name CB) 7.92 0.29 0.29
55 assign (segid 3A4 and resid 122 and name CA) (segid 3A4 and resid 264 and name C) 7.41 0.27 0.27
assign (segid 3A4 and resid 122 and name CA) (segid 3A4 and resid 264 and name CA) 6.16 0.22 0.23
assign (segid 3A4 and resid 122 and name CA) (segid 3A4 and resid 264 and name N) 6.70 0.23 0.22
60 assign (segid 3A4 and resid 122 and name CA) (segid 3A4 and resid 265 and name CA) 9.65 0.34 0.33
assign (segid 3A4 and resid 122 and name CA) (segid 3A4 and resid 266 and name CA) 11.38 0.13 0.13
assign (segid 3A4 and resid 122 and name CA) (segid 3A4 and resid 267 and name CA) 9.95 0.31 0.30
65 assign (segid 3A4 and resid 122 and name CA) (segid 3A4 and resid 267 and name CB) 8.69 0.34 0.34
assign (segid 3A4 and resid 122 and name CA) (segid 3A4 and resid 268 and name CA) 10.74 0.35 0.36
70 assign (segid 3A4 and resid 122 and name CA) (segid 3A4 and resid 268 and name CB) 10.41 0.37 0.36
assign (segid 3A4 and resid 122 and name CA) (segid 3A4 and resid 269 and name CA) 14.07 0.28 0.28
75 assign (segid 3A4 and resid 122 and name CA) (segid 3A4 and resid 270 and name CA) 14.91 0.34 0.34
assign (segid 3A4 and resid 122 and name CA) (segid 3A4 and resid 270 and name CB) 14.47 0.30 0.30
80 assign (segid 3A4 and resid 122 and name CA) (segid 3A4 and resid 271 and name CA) 14.28 0.50 0.50
assign (segid 3A4 and resid 122 and name CA) (segid 3A4 and resid 271 and name CB) 13.06 0.51 0.52
assign (segid 3A4 and resid 122 and name CA) (segid 3A4 and resid 272 and name CA) 16.51 0.40 0.39
assign (segid 3A4 and resid 122 and name CA) (segid 3A4 and resid 272 and name CB) 16.24 0.41 0.41
70 assign (segid 3A4 and resid 122 and name CA) (segid 3A4 and resid 277 and name CA) 18.91 0.26 0.27
assign (segid 3A4 and resid 122 and name CA) (segid 3A4 and resid 277 and name CB) 18.15 0.24 0.24
65 assign (segid 3A4 and resid 122 and name CA) (segid 3A4 and resid 309 and name CA) 17.45 0.93 0.93
assign (segid 3A4 and resid 122 and name CA) (segid 3A4 and resid 309 and name CB) 17.55 0.95 0.96
70 assign (segid 3A4 and resid 122 and name CA) (segid 3A4 and resid 312 and name CA) 16.29 0.96 0.97
assign (segid 3A4 and resid 122 and name CA) (segid 3A4 and resid 312 and name CB) 15.19 0.95 0.94
75 assign (segid 3A4 and resid 122 and name CA) (segid 3A4 and resid 313 and name CA) 17.04 0.79 0.79
assign (segid 3A4 and resid 122 and name CA) (segid 3A4 and resid 313 and name CB) 17.62 0.74 0.75
80 assign (segid 3A4 and resid 122 and name CA) (segid 3A4 and resid 315 and name CB) 18.40 0.91 0.91
assign (segid 3A4 and resid 122 and name CA) (segid 3A4 and resid 316 and name CA) 15.69 0.88 0.88
75 assign (segid 3A4 and resid 122 and name CA) (segid 3A4 and resid 317 and name CA) 17.21 0.89 0.88
80 assign (segid 3A4 and resid 122 and name CA) (segid 3A4 and resid 318 and name CA) 14.77 0.94 0.95
assign (segid 3A4 and resid 122 and name CA) (segid 3A4 and resid 318 and name CB) 13.70 1.00 1.01
assign (segid 3A4 and resid 122 and name CA) (segid 3A4 and resid 319 and name CA) 17.61 0.89 0.90
assign (segid 3A4 and resid 122 and name CA) (segid 3A4 and resid 319 and name CB) 18.13 0.86 0.86
80 assign (segid 3A4 and resid 122 and name CA) (segid 3A4 and resid 397 and name CA) 16.71 0.46 0.46
assign (segid 3A4 and resid 122 and name CA) (segid 3A4 and resid 397 and name CB) 16.76 0.52 0.52
assign (segid 3A4 and resid 122 and name CA) (segid 3A4 and resid 398 and name CA) 18.23 0.56 0.56
assign (segid 3A4 and resid 122 and name CA) (segid 3A4 and resid 399 and name CA) 18.79 0.38 0.37
assign (segid 3A4 and resid 122 and name CA) (segid 3A4 and resid 400 and name CA) 15.29 0.43 0.44

	assign (segid 3A4 and resid 122 and name CB)	(segid 3A4 and resid 156 and name CB)	16.60	1.23	1.23
	assign (segid 3A4 and resid 122 and name CB)	(segid 3A4 and resid 157 and name CA)	14.31	1.16	1.16
	assign (segid 3A4 and resid 122 and name CB)	(segid 3A4 and resid 157 and name CB)	13.62	1.36	1.37
	assign (segid 3A4 and resid 122 and name CB)	(segid 3A4 and resid 158 and name CA)	13.68	2.38	2.39
	assign (segid 3A4 and resid 122 and name CB)	(segid 3A4 and resid 160 and name CA)	17.14	1.29	1.29
5	assign (segid 3A4 and resid 122 and name CB)	(segid 3A4 and resid 160 and name CB)	17.07	1.53	1.53
	assign (segid 3A4 and resid 122 and name CB)	(segid 3A4 and resid 252 and name CA)	17.95	0.60	0.60
	assign (segid 3A4 and resid 122 and name CB)	(segid 3A4 and resid 252 and name CB)	18.39	0.65	0.65
	assign (segid 3A4 and resid 122 and name CB)	(segid 3A4 and resid 253 and name CA)	16.60	0.33	0.33
	assign (segid 3A4 and resid 122 and name CB)	(segid 3A4 and resid 254 and name CA)	17.13	0.43	0.44
10	assign (segid 3A4 and resid 122 and name CB)	(segid 3A4 and resid 255 and name CA)	15.71	0.58	0.58
	assign (segid 3A4 and resid 122 and name CB)	(segid 3A4 and resid 256 and name CA)	12.48	0.46	0.47
	assign (segid 3A4 and resid 122 and name CB)	(segid 3A4 and resid 257 and name CA)	10.65	0.78	0.77
	assign (segid 3A4 and resid 122 and name CB)	(segid 3A4 and resid 258 and name CA)	12.06	0.53	0.53
	assign (segid 3A4 and resid 122 and name CB)	(segid 3A4 and resid 258 and name CB)	13.58	0.52	0.53
15	assign (segid 3A4 and resid 122 and name CB)	(segid 3A4 and resid 259 and name CA)	11.36	0.48	0.47
	assign (segid 3A4 and resid 122 and name CB)	(segid 3A4 and resid 259 and name CB)	12.09	0.48	0.47
	assign (segid 3A4 and resid 122 and name CB)	(segid 3A4 and resid 260 and name CA)	7.66	0.48	0.48
	assign (segid 3A4 and resid 122 and name CB)	(segid 3A4 and resid 260 and name CB)	7.16	0.53	0.54
	assign (segid 3A4 and resid 122 and name CB)	(segid 3A4 and resid 260 and name O)	6.52	0.48	0.48
20	assign (segid 3A4 and resid 122 and name CB)	(segid 3A4 and resid 261 and name CA)	7.69	0.52	0.52
	assign (segid 3A4 and resid 122 and name CB)	(segid 3A4 and resid 262 and name CA)	10.35	0.38	0.39
	assign (segid 3A4 and resid 122 and name CB)	(segid 3A4 and resid 262 and name CB)	11.59	0.39	0.39
	assign (segid 3A4 and resid 122 and name CB)	(segid 3A4 and resid 263 and name CA)	8.98	0.40	0.40
	assign (segid 3A4 and resid 122 and name CB)	(segid 3A4 and resid 263 and name CB)	8.67	0.48	0.48
25	assign (segid 3A4 and resid 122 and name CB)	(segid 3A4 and resid 264 and name C)	7.41	0.24	0.25
	assign (segid 3A4 and resid 122 and name CB)	(segid 3A4 and resid 264 and name CA)	6.32	0.26	0.27
	assign (segid 3A4 and resid 122 and name CB)	(segid 3A4 and resid 264 and name N)	7.01	0.33	0.32
	assign (segid 3A4 and resid 122 and name CB)	(segid 3A4 and resid 265 and name CA)	9.46	0.29	0.28
	assign (segid 3A4 and resid 122 and name CB)	(segid 3A4 and resid 266 and name CA)	11.65	0.27	0.27
30	assign (segid 3A4 and resid 122 and name CB)	(segid 3A4 and resid 267 and name CA)	10.39	0.44	0.44
	assign (segid 3A4 and resid 122 and name CB)	(segid 3A4 and resid 267 and name CB)	9.26	0.48	0.47
	assign (segid 3A4 and resid 122 and name CB)	(segid 3A4 and resid 268 and name CA)	10.68	0.40	0.41
	assign (segid 3A4 and resid 122 and name CB)	(segid 3A4 and resid 268 and name CB)	10.15	0.39	0.38
	assign (segid 3A4 and resid 122 and name CB)	(segid 3A4 and resid 269 and name CA)	14.05	0.35	0.36
35	assign (segid 3A4 and resid 122 and name CB)	(segid 3A4 and resid 270 and name CA)	15.25	0.40	0.40
	assign (segid 3A4 and resid 122 and name CB)	(segid 3A4 and resid 270 and name CB)	14.95	0.37	0.37
	assign (segid 3A4 and resid 122 and name CB)	(segid 3A4 and resid 271 and name CA)	14.52	0.52	0.52
	assign (segid 3A4 and resid 122 and name CB)	(segid 3A4 and resid 271 and name CB)	13.27	0.53	0.52
	assign (segid 3A4 and resid 122 and name CB)	(segid 3A4 and resid 272 and name CA)	16.46	0.40	0.39
40	assign (segid 3A4 and resid 122 and name CB)	(segid 3A4 and resid 272 and name CB)	16.08	0.41	0.41
	assign (segid 3A4 and resid 122 and name CB)	(segid 3A4 and resid 277 and name CB)	18.76	0.30	0.30
	assign (segid 3A4 and resid 122 and name CB)	(segid 3A4 and resid 309 and name CA)	17.93	1.04	1.03
	assign (segid 3A4 and resid 122 and name CB)	(segid 3A4 and resid 309 and name CB)	18.11	1.05	1.04
	assign (segid 3A4 and resid 122 and name CB)	(segid 3A4 and resid 312 and name CA)	16.36	1.08	1.08
45	assign (segid 3A4 and resid 122 and name CB)	(segid 3A4 and resid 312 and name CB)	15.36	1.07	1.06
	assign (segid 3A4 and resid 122 and name CB)	(segid 3A4 and resid 313 and name CA)	17.00	0.91	0.92
	assign (segid 3A4 and resid 122 and name CB)	(segid 3A4 and resid 313 and name CB)	17.67	0.87	0.87
	assign (segid 3A4 and resid 122 and name CB)	(segid 3A4 and resid 315 and name CA)	18.38	1.01	1.00
	assign (segid 3A4 and resid 122 and name CB)	(segid 3A4 and resid 315 and name CB)	18.11	1.04	1.05
50	assign (segid 3A4 and resid 122 and name CB)	(segid 3A4 and resid 316 and name CA)	15.22	0.96	0.97
	assign (segid 3A4 and resid 122 and name CB)	(segid 3A4 and resid 317 and name CA)	16.73	0.99	0.98
	assign (segid 3A4 and resid 122 and name CB)	(segid 3A4 and resid 318 and name CA)	14.20	1.02	1.02
	assign (segid 3A4 and resid 122 and name CB)	(segid 3A4 and resid 318 and name CB)	13.23	1.11	1.10
	assign (segid 3A4 and resid 122 and name CB)	(segid 3A4 and resid 319 and name CA)	16.99	0.96	0.96
55	assign (segid 3A4 and resid 122 and name CB)	(segid 3A4 and resid 319 and name CB)	17.60	0.90	0.89
	assign (segid 3A4 and resid 122 and name CB)	(segid 3A4 and resid 397 and name CA)	17.27	0.58	0.58
	assign (segid 3A4 and resid 122 and name CB)	(segid 3A4 and resid 397 and name CB)	17.20	0.62	0.62
	assign (segid 3A4 and resid 122 and name CB)	(segid 3A4 and resid 400 and name CA)	16.26	0.54	0.53
	assign (segid 3A4 and resid 122 and name CB)	(segid 3A4 and resid 400 and name CB)	15.51	0.54	0.53
60	assign (segid 3A4 and resid 122 and name CB)	(segid 3A4 and resid 401 and name CA)	14.94	0.63	0.63
	assign (segid 3A4 and resid 122 and name CB)	(segid 3A4 and resid 402 and name CA)	18.02	0.64	0.64
	assign (segid 3A4 and resid 122 and name CB)	(segid 3A4 and resid 403 and name CA)	18.03	0.65	0.65
	assign (segid 3A4 and resid 122 and name CB)	(segid 3A4 and resid 403 and name CB)	18.29	0.74	0.74
	assign (segid 3A4 and resid 122 and name CB)	(segid 3A4 and resid 404 and name CA)	14.55	0.67	0.66
65	assign (segid 3A4 and resid 122 and name CB)	(segid 3A4 and resid 404 and name CB)	13.27	0.65	0.65
	assign (segid 3A4 and resid 122 and name CB)	(segid 3A4 and resid 405 and name CA)	15.14	0.66	0.67
	assign (segid 3A4 and resid 122 and name CB)	(segid 3A4 and resid 405 and name CB)	15.36	0.71	0.71
	assign (segid 3A4 and resid 122 and name CB)	(segid 3A4 and resid 406 and name CA)	18.63	0.64	0.64
	assign (segid 3A4 and resid 122 and name CB)	(segid 3A4 and resid 407 and name CA)	17.84	0.72	0.73
70	assign (segid 3A4 and resid 122 and name CB)	(segid 3A4 and resid 407 and name CB)	17.58	0.82	0.82
	assign (segid 3A4 and resid 122 and name CB)	(segid 3A4 and resid 408 and name CA)	15.09	0.76	0.75
	assign (segid 3A4 and resid 122 and name CB)	(segid 3A4 and resid 408 and name CB)	13.75	0.69	0.69
	assign (segid 3A4 and resid 122 and name CB)	(segid 3A4 and resid 409 and name CA)	17.36	0.73	0.73
	assign (segid 3A4 and resid 122 and name CB)	(segid 3A4 and resid 409 and name CB)	17.70	0.75	0.75
75	assign (segid 3A4 and resid 122 and name CB)	(segid 3A4 and resid 411 and name CB)	18.30	0.96	0.95
	assign (segid 3A4 and resid 122 and name CB)	(segid 3A4 and resid 412 and name CA)	17.54	0.52	0.51
	assign (segid 3A4 and resid 122 and name CB)	(segid 3A4 and resid 413 and name CA)	18.07	0.92	0.92
	assign (segid 3A4 and resid 122 and name CB)	(segid 3A4 and resid 414 and name CA)	15.05	0.50	0.49
	assign (segid 3A4 and resid 122 and name CB)	(segid 3A4 and resid 415 and name CA)	14.62	1.16	1.16
80	assign (segid 3A4 and resid 122 and name CB)	(segid 3A4 and resid 415 and name CB)	15.59	1.41	1.42
	assign (segid 3A4 and resid 122 and name CB)	(segid 3A4 and resid 416 and name CA)	13.23	0.99	1.00
	assign (segid 3A4 and resid 122 and name CB)	(segid 3A4 and resid 417 and name CA)	14.74	1.37	1.38

	assign (segid 3A4 and resid 122 and name CB) (segid 3A4 and resid 423 and name CA) 13.69 1.00 1.00
	assign (segid 3A4 and resid 122 and name CB) (segid 3A4 and resid 424 and name CA) 11.99 1.53 1.54
	assign (segid 3A4 and resid 122 and name CB) (segid 3A4 and resid 425 and name CA) 11.21 1.80 1.80
	assign (segid 3A4 and resid 122 and name CB) (segid 3A4 and resid 426 and name CA) 11.18 1.20 1.19
5	assign (segid 3A4 and resid 122 and name CB) (segid 3A4 and resid 427 and name CA) 11.39 1.23 1.24
	assign (segid 3A4 and resid 122 and name CB) (segid 3A4 and resid 428 and name CA) 13.56 1.91 1.91
	assign (segid 3A4 and resid 122 and name CB) (segid 3A4 and resid 429 and name CA) 15.05 1.54 1.54
	assign (segid 3A4 and resid 122 and name CB) (segid 3A4 and resid 430 and name CA) 17.17 1.98 1.98
	assign (segid 3A4 and resid 122 and name CB) (segid 3A4 and resid 431 and name CA) 17.04 1.10 1.09
10	assign (segid 3A4 and resid 122 and name CB) (segid 3A4 and resid 433 and name CA) 12.32 1.14 1.14
	assign (segid 3A4 and resid 122 and name CB) (segid 3A4 and resid 434 and name CA) 8.93 1.18 1.18
	assign (segid 3A4 and resid 122 and name CB) (segid 3A4 and resid 435 and name CA) 6.96 1.06 1.05
	assign (segid 3A4 and resid 122 and name CB) (segid 3A4 and resid 436 and name CA) 6.22 1.39 1.39
	assign (segid 3A4 and resid 122 and name CB) (segid 3A4 and resid 436 and name O) 5.02 1.40 1.40
15	assign (segid 3A4 and resid 122 and name CB) (segid 3A4 and resid 437 and name CA) 5.29 1.12 1.12
	assign (segid 3A4 and resid 122 and name CB) (segid 3A4 and resid 438 and name C) 6.41 0.58 0.58
	assign (segid 3A4 and resid 122 and name CB) (segid 3A4 and resid 438 and name CA) 6.05 0.91 0.91
	assign (segid 3A4 and resid 122 and name CB) (segid 3A4 and resid 438 and name N) 5.18 0.96 0.97
	assign (segid 3A4 and resid 122 and name CB) (segid 3A4 and resid 438 and name O) 5.90 0.35 0.35
20	assign (segid 3A4 and resid 122 and name CB) (segid 3A4 and resid 439 and name CA) 8.29 0.32 0.33
	assign (segid 3A4 and resid 122 and name CB) (segid 3A4 and resid 440 and name CA) 10.40 0.41 0.41
	assign (segid 3A4 and resid 122 and name N) (segid 3A4 and resid 122 and name C) 2.46 0.02 0.03
	assign (segid 3A4 and resid 122 and name N) (segid 3A4 and resid 122 and name CA) 1.46 0.02 0.01
	assign (segid 3A4 and resid 122 and name N) (segid 3A4 and resid 122 and name CB) 2.46 0.07 0.06
25	assign (segid 3A4 and resid 122 and name N) (segid 3A4 and resid 122 and name O) 3.44 0.08 0.08
	assign (segid 3A4 and resid 122 and name N) (segid 3A4 and resid 123 and name C) 4.82 0.09 0.08
	assign (segid 3A4 and resid 122 and name N) (segid 3A4 and resid 123 and name CA) 4.29 0.06 0.06
	assign (segid 3A4 and resid 122 and name N) (segid 3A4 and resid 123 and name CB) 5.12 0.12 0.11
	assign (segid 3A4 and resid 122 and name N) (segid 3A4 and resid 123 and name N) 2.89 0.06 0.06
30	assign (segid 3A4 and resid 122 and name N) (segid 3A4 and resid 123 and name O) 5.87 0.15 0.14
	assign (segid 3A4 and resid 122 and name N) (segid 3A4 and resid 124 and name C) 5.70 0.19 0.18
	assign (segid 3A4 and resid 122 and name N) (segid 3A4 and resid 124 and name CA) 5.54 0.24 0.24
	assign (segid 3A4 and resid 122 and name N) (segid 3A4 and resid 124 and name CB) 5.87 0.26 0.27
	assign (segid 3A4 and resid 122 and name N) (segid 3A4 and resid 124 and name N) 4.52 0.22 0.22
35	assign (segid 3A4 and resid 122 and name N) (segid 3A4 and resid 124 and name O) 6.86 0.18 0.19
	assign (segid 3A4 and resid 122 and name N) (segid 3A4 and resid 125 and name C) 5.83 0.29 0.28
	assign (segid 3A4 and resid 122 and name N) (segid 3A4 and resid 125 and name CA) 5.57 0.12 0.11
	assign (segid 3A4 and resid 122 and name N) (segid 3A4 and resid 125 and name CB) 5.38 0.31 0.32
	assign (segid 3A4 and resid 122 and name N) (segid 3A4 and resid 125 and name N) 4.84 0.13 0.14
40	assign (segid 3A4 and resid 122 and name N) (segid 3A4 and resid 125 and name O) 6.91 0.28 0.28
	assign (segid 3A4 and resid 122 and name N) (segid 3A4 and resid 126 and name CA) 5.92 0.76 0.76
	assign (segid 3A4 and resid 122 and name N) (segid 3A4 and resid 126 and name N) 5.16 0.55 0.56
	assign (segid 3A4 and resid 122 and name N) (segid 3A4 and resid 260 and name O) 7.16 0.41 0.42
	assign (segid 3A4 and resid 122 and name N) (segid 3A4 and resid 263 and name C) 7.73 0.20 0.19
45	assign (segid 3A4 and resid 122 and name N) (segid 3A4 and resid 264 and name C) 7.39 0.31 0.31
	assign (segid 3A4 and resid 122 and name N) (segid 3A4 and resid 264 and name CA) 6.24 0.28 0.29
	assign (segid 3A4 and resid 122 and name N) (segid 3A4 and resid 264 and name N) 6.94 0.26 0.27
	assign (segid 3A4 and resid 122 and name N) (segid 3A4 and resid 438 and name C) 5.57 0.66 0.66
	assign (segid 3A4 and resid 122 and name N) (segid 3A4 and resid 438 and name N) 5.30 0.92 0.93
50	assign (segid 3A4 and resid 122 and name N) (segid 3A4 and resid 438 and name O) 4.72 0.53 0.54
	assign (segid 3A4 and resid 122 and name N) (segid 3A4 and resid 439 and name CA) 7.12 0.33 0.33
	assign (segid 3A4 and resid 122 and name O) (segid 3A4 and resid 122 and name CB) 3.42 0.09 0.08
	assign (segid 3A4 and resid 122 and name O) (segid 3A4 and resid 123 and name C) 3.10 0.06 0.05
	assign (segid 3A4 and resid 122 and name O) (segid 3A4 and resid 123 and name CA) 2.77 0.04 0.04
55	assign (segid 3A4 and resid 122 and name O) (segid 3A4 and resid 123 and name CB) 4.24 0.06 0.06
	assign (segid 3A4 and resid 122 and name O) (segid 3A4 and resid 123 and name N) 2.26 0.01 0.01
	assign (segid 3A4 and resid 122 and name O) (segid 3A4 and resid 123 and name O) 3.58 0.22 0.22
	assign (segid 3A4 and resid 122 and name O) (segid 3A4 and resid 124 and name C) 4.44 0.30 0.31
	assign (segid 3A4 and resid 122 and name O) (segid 3A4 and resid 124 and name CA) 4.58 0.26 0.27
60	assign (segid 3A4 and resid 122 and name O) (segid 3A4 and resid 124 and name CB) 5.73 0.26 0.27
	assign (segid 3A4 and resid 122 and name O) (segid 3A4 and resid 124 and name N) 3.60 0.25 0.24
	assign (segid 3A4 and resid 122 and name O) (segid 3A4 and resid 124 and name O) 5.48 0.31 0.30
	assign (segid 3A4 and resid 122 and name O) (segid 3A4 and resid 125 and name C) 3.93 0.29 0.29
	assign (segid 3A4 and resid 122 and name O) (segid 3A4 and resid 125 and name CA) 4.24 0.32 0.32
65	assign (segid 3A4 and resid 122 and name O) (segid 3A4 and resid 125 and name CB) 4.87 0.55 0.54
	assign (segid 3A4 and resid 122 and name O) (segid 3A4 and resid 125 and name N) 3.60 0.33 0.34
	assign (segid 3A4 and resid 122 and name O) (segid 3A4 and resid 125 and name O) 4.73 0.33 0.34
	assign (segid 3A4 and resid 122 and name O) (segid 3A4 and resid 126 and name C) 4.19 0.57 0.57
	assign (segid 3A4 and resid 122 and name O) (segid 3A4 and resid 126 and name CA) 3.89 0.15 0.14
70	assign (segid 3A4 and resid 122 and name O) (segid 3A4 and resid 126 and name N) 3.34 0.25 0.24
	assign (segid 3A4 and resid 122 and name O) (segid 3A4 and resid 126 and name O) 5.30 0.53 0.54
	assign (segid 3A4 and resid 122 and name O) (segid 3A4 and resid 127 and name C) 5.73 1.09 1.10
	assign (segid 3A4 and resid 122 and name O) (segid 3A4 and resid 127 and name CA) 4.66 1.17 1.16
	assign (segid 3A4 and resid 122 and name O) (segid 3A4 and resid 127 and name CB) 4.53 1.41 1.40
75	assign (segid 3A4 and resid 122 and name O) (segid 3A4 and resid 127 and name N) 3.66 0.95 0.96
	assign (segid 3A4 and resid 122 and name O) (segid 3A4 and resid 128 and name N) 5.68 1.03 1.04
	assign (segid 3A4 and resid 122 and name O) (segid 3A4 and resid 260 and name C) 6.98 0.55 0.55
	assign (segid 3A4 and resid 122 and name O) (segid 3A4 and resid 260 and name CA) 6.83 0.45 0.46
	assign (segid 3A4 and resid 122 and name O) (segid 3A4 and resid 260 and name CB) 6.17 0.62 0.63
80	assign (segid 3A4 and resid 122 and name O) (segid 3A4 and resid 260 and name O) 6.56 0.51 0.51
	assign (segid 3A4 and resid 123 and name C) (segid 3A4 and resid 123 and name CB) 2.50 0.03 0.02
	assign (segid 3A4 and resid 123 and name C) (segid 3A4 and resid 123 and name O) 1.24 0.02 0.01
	assign (segid 3A4 and resid 123 and name C) (segid 3A4 and resid 124 and name C) 3.22 0.11 0.11

	assign (segid 3A4 and resid 123 and name C) (segid 3A4 and resid 124 and name CA)	2.44	0.02	0.01
	assign (segid 3A4 and resid 123 and name C) (segid 3A4 and resid 124 and name CB)	3.68	0.03	0.02
	assign (segid 3A4 and resid 123 and name C) (segid 3A4 and resid 124 and name N)	1.33	0.01	0.00
	assign (segid 3A4 and resid 123 and name C) (segid 3A4 and resid 124 and name O)	4.21	0.14	0.15
	assign (segid 3A4 and resid 123 and name C) (segid 3A4 and resid 125 and name C)	5.04	0.32	0.31
5	assign (segid 3A4 and resid 123 and name C) (segid 3A4 and resid 125 and name CA)	4.69	0.19	0.19
	assign (segid 3A4 and resid 123 and name C) (segid 3A4 and resid 125 and name CB)	5.65	0.30	0.29
	assign (segid 3A4 and resid 123 and name C) (segid 3A4 and resid 125 and name N)	3.39	0.14	0.14
	assign (segid 3A4 and resid 123 and name C) (segid 3A4 and resid 125 and name O)	5.84	0.10	0.10
	assign (segid 3A4 and resid 123 and name C) (segid 3A4 and resid 126 and name C)	5.80	0.52	0.51
10	assign (segid 3A4 and resid 123 and name C) (segid 3A4 and resid 126 and name CA)	5.78	0.70	0.70
	assign (segid 3A4 and resid 123 and name C) (segid 3A4 and resid 126 and name N)	4.86	0.68	0.67
	assign (segid 3A4 and resid 123 and name C) (segid 3A4 and resid 126 and name O)	6.94	0.49	0.49
	assign (segid 3A4 and resid 123 and name C) (segid 3A4 and resid 127 and name C)	6.24	0.23	0.24
	assign (segid 3A4 and resid 123 and name C) (segid 3A4 and resid 127 and name CA)	5.45	0.18	0.18
	assign (segid 3A4 and resid 123 and name C) (segid 3A4 and resid 127 and name CB)	4.82	0.08	0.08
15	assign (segid 3A4 and resid 123 and name C) (segid 3A4 and resid 127 and name N)	4.88	0.36	0.35
	assign (segid 3A4 and resid 123 and name C) (segid 3A4 and resid 127 and name O)	7.42	0.20	0.20
	assign (segid 3A4 and resid 123 and name C) (segid 3A4 and resid 128 and name C)	6.96	0.55	0.55
	assign (segid 3A4 and resid 123 and name C) (segid 3A4 and resid 128 and name CA)	6.66	0.77	0.77
20	assign (segid 3A4 and resid 123 and name C) (segid 3A4 and resid 128 and name N)	5.88	0.44	0.43
	assign (segid 3A4 and resid 123 and name C) (segid 3A4 and resid 128 and name O)	1.52	0.02	0.01
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 123 and name CB)	1.53	0.02	0.01
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 123 and name N)	2.39	0.03	0.02
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 123 and name O)	4.57	0.09	0.08
25	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 124 and name C)	3.81	0.01	0.01
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 124 and name CA)	4.85	0.06	0.05
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 124 and name CB)	2.44	0.02	0.03
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 124 and name N)	5.64	0.13	0.12
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 124 and name O)	5.82	0.22	0.21
30	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 125 and name C)	5.67	0.15	0.16
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 125 and name CA)	6.47	0.36	0.36
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 125 and name CB)	4.45	0.09	0.10
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 125 and name N)	6.64	0.11	0.11
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 125 and name O)	6.15	0.19	0.18
35	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 126 and name C)	6.11	0.48	0.47
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 126 and name CA)	5.39	0.49	0.50
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 126 and name N)	7.25	0.17	0.16
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 126 and name O)	6.82	0.50	0.51
40	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 127 and name C)	5.81	0.36	0.36
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 127 and name CA)	5.07	0.65	0.65
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 127 and name N)	5.28	0.12	0.11
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 127 and name O)	7.88	0.70	0.70
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 128 and name C)	7.75	0.85	0.86
45	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 128 and name N)	6.68	0.63	0.62
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 128 and name O)	10.11	0.30	0.31
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 129 and name C)	10.09	0.18	0.17
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 129 and name CA)	11.45	0.40	0.40
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 130 and name C)	11.02	0.60	0.60
50	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 131 and name C)	11.87	0.54	0.53
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 131 and name CA)	11.05	0.75	0.75
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 132 and name C)	13.60	0.73	0.73
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 132 and name CA)	13.26	0.78	0.77
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 133 and name C)	15.74	0.38	0.38
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 133 and name CA)	15.51	0.28	0.29
55	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 134 and name C)	16.64	0.34	0.35
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 135 and name C)	17.49	0.71	0.71
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 135 and name CA)	16.71	0.89	0.88
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 135 and name CB)	16.43	1.38	1.39
60	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 147 and name C)	17.00	1.39	1.39
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 147 and name CA)	17.15	1.21	1.20
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 148 and name C)	15.65	1.81	1.82
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 149 and name C)	16.08	2.49	2.49
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 149 and name CA)	13.04	1.33	1.32
65	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 151 and name C)	13.06	1.71	1.70
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 152 and name C)	14.66	1.14	1.14
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 152 and name CA)	15.51	1.29	1.29
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 153 and name C)	13.63	1.49	1.49
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 153 and name CA)	13.48	2.05	2.06
70	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 154 and name C)	11.98	1.52	1.53
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 155 and name C)	13.70	2.27	2.28
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 155 and name CA)	14.32	2.38	2.39
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 156 and name C)	15.32	1.33	1.33
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 156 and name CA)	15.62	1.41	1.41
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 157 and name C)	14.14	1.41	1.41
75	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 157 and name CA)	13.39	1.51	1.51
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 160 and name C)	17.58	1.48	1.49
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 252 and name C)	17.44	0.88	0.88
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 252 and name CA)	17.61	0.96	0.96
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 253 and name C)	16.77	0.58	0.58
80	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 253 and name CA)	18.00	0.64	0.63
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 254 and name C)	16.24	0.64	0.64
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 255 and name C)	12.71	0.61	0.61

	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 257 and name CA)	11.94	0.76	0.76
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 258 and name CA)	14.13	0.48	0.49
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 258 and name CB)	15.59	0.50	0.50
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 259 and name CA)	13.00	0.36	0.35
5	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 259 and name CB)	13.27	0.39	0.38
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 260 and name CA)	9.32	0.37	0.37
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 260 and name CB)	8.48	0.52	0.52
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 261 and name CA)	10.84	0.57	0.56
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 262 and name CA)	13.39	0.45	0.44
10	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 262 and name CB)	14.35	0.44	0.43
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 263 and name CA)	11.44	0.27	0.28
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 263 and name CB)	10.60	0.26	0.26
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 264 and name CA)	9.76	0.34	0.34
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 265 and name CA)	13.33	0.37	0.38
15	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 266 and name CA)	14.91	0.25	0.25
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 267 and name CA)	13.33	0.26	0.25
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 267 and name CB)	11.95	0.22	0.23
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 268 and name CA)	14.31	0.38	0.39
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 268 and name CB)	14.04	0.37	0.37
20	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 269 and name CA)	17.71	0.31	0.31
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 270 and name CA)	18.28	0.40	0.40
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 270 and name CB)	17.73	0.36	0.36
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 271 and name CA)	17.45	0.57	0.58
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 271 and name CB)	16.19	0.60	0.60
25	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 312 and name CB)	18.64	0.83	0.82
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 318 and name CA)	17.62	0.95	0.94
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 318 and name CB)	16.50	0.96	0.96
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 397 and name CA)	18.44	0.44	0.44
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 397 and name CB)	18.63	0.51	0.51
30	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 400 and name CA)	16.73	0.50	0.50
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 400 and name CB)	15.93	0.53	0.52
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 401 and name CA)	16.29	0.40	0.39
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 402 and name CA)	19.24	0.39	0.39
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 403 and name CA)	18.39	0.45	0.45
35	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 403 and name CB)	18.38	0.54	0.55
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 404 and name CA)	14.93	0.42	0.42
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 404 and name CB)	13.78	0.40	0.40
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 405 and name CA)	16.35	0.73	0.73
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 405 and name CB)	16.92	0.72	0.72
40	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 407 and name CA)	17.84	0.53	0.54
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 407 and name CB)	17.30	0.54	0.53
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 408 and name CA)	15.37	0.58	0.58
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 408 and name CB)	14.30	0.53	0.52
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 409 and name CA)	18.24	0.50	0.50
45	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 409 and name CB)	18.89	0.55	0.54
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 411 and name CA)	18.79	0.52	0.51
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 411 and name CB)	17.75	0.62	0.62
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 412 and name CA)	17.72	0.46	0.45
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 413 and name CA)	19.04	0.79	0.79
50	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 414 and name CA)	16.44	0.23	0.24
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 415 and name CA)	16.50	0.84	0.84
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 415 and name CB)	17.44	0.96	0.96
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 416 and name CA)	15.43	0.87	0.87
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 417 and name CA)	16.52	1.44	1.43
55	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 423 and name CA)	16.85	1.44	1.44
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 424 and name CA)	15.59	1.69	1.69
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 426 and name CA)	15.08	1.36	1.35
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 427 and name CA)	15.12	1.36	1.36
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 428 and name CA)	16.93	1.78	1.78
60	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 433 and name CA)	15.93	1.18	1.18
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 434 and name CA)	12.85	1.09	1.09
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 435 and name CA)	11.19	1.02	1.02
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 436 and name CA)	9.72	1.79	1.80
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 437 and name CA)	8.36	1.46	1.46
65	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 438 and name CA)	9.21	1.09	1.08
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 439 and name CA)	9.94	0.63	0.62
	assign (segid 3A4 and resid 123 and name CA) (segid 3A4 and resid 440 and name CA)	11.71	0.41	0.41
	assign (segid 3A4 and resid 123 and name CB) (segid 3A4 and resid 124 and name C)	5.58	0.16	0.16
	assign (segid 3A4 and resid 123 and name CB) (segid 3A4 and resid 124 and name CA)	4.50	0.15	0.14
70	assign (segid 3A4 and resid 123 and name CB) (segid 3A4 and resid 124 and name CB)	5.26	0.17	0.18
	assign (segid 3A4 and resid 123 and name CB) (segid 3A4 and resid 124 and name N)	3.18	0.16	0.16
	assign (segid 3A4 and resid 123 and name CB) (segid 3A4 and resid 124 and name O)	6.60	0.18	0.18
	assign (segid 3A4 and resid 123 and name CB) (segid 3A4 and resid 125 and name C)	7.26	0.24	0.24
	assign (segid 3A4 and resid 123 and name CB) (segid 3A4 and resid 125 and name CA)	7.00	0.19	0.19
75	assign (segid 3A4 and resid 123 and name CB) (segid 3A4 and resid 125 and name CB)	7.77	0.36	0.36
	assign (segid 3A4 and resid 123 and name CB) (segid 3A4 and resid 125 and name N)	5.68	0.16	0.17
	assign (segid 3A4 and resid 123 and name CB) (segid 3A4 and resid 126 and name C)	7.52	0.30	0.30
	assign (segid 3A4 and resid 123 and name CB) (segid 3A4 and resid 126 and name CA)	7.55	0.52	0.52
	assign (segid 3A4 and resid 123 and name CB) (segid 3A4 and resid 126 and name N)	6.85	0.52	0.52
80	assign (segid 3A4 and resid 123 and name CB) (segid 3A4 and resid 127 and name CA)	6.96	0.19	0.19
	assign (segid 3A4 and resid 123 and name CB) (segid 3A4 and resid 127 and name CB)	6.02	0.42	0.43
	assign (segid 3A4 and resid 123 and name CB) (segid 3A4 and resid 127 and name N)	6.58	0.11	0.12
	assign (segid 3A4 and resid 123 and name CB) (segid 3A4 and resid 128 and name CA)	9.00	0.64	0.64

	assign (segid 3A4 and resid 123 and name CB)	(segid 3A4 and resid 128 and name CB)	8.85	0.84	0.83
	assign (segid 3A4 and resid 123 and name CB)	(segid 3A4 and resid 129 and name CA)	11.47	0.29	0.29
	assign (segid 3A4 and resid 123 and name CB)	(segid 3A4 and resid 129 and name CB)	11.51	0.70	0.19
	assign (segid 3A4 and resid 123 and name CB)	(segid 3A4 and resid 130 and name CA)	12.70	0.53	0.53
5	assign (segid 3A4 and resid 123 and name CB)	(segid 3A4 and resid 130 and name CB)	12.24	0.77	0.77
	assign (segid 3A4 and resid 123 and name CB)	(segid 3A4 and resid 131 and name CA)	12.89	0.49	0.48
	assign (segid 3A4 and resid 123 and name CB)	(segid 3A4 and resid 131 and name CB)	11.98	0.67	0.67
	assign (segid 3A4 and resid 123 and name CB)	(segid 3A4 and resid 132 and name CA)	14.68	0.76	0.76
	assign (segid 3A4 and resid 123 and name CB)	(segid 3A4 and resid 132 and name CB)	14.37	0.83	0.83
10	assign (segid 3A4 and resid 123 and name CB)	(segid 3A4 and resid 133 and name CA)	16.95	0.40	0.40
	assign (segid 3A4 and resid 123 and name CB)	(segid 3A4 and resid 133 and name CB)	16.78	0.31	0.30
	assign (segid 3A4 and resid 123 and name CB)	(segid 3A4 and resid 134 and name CA)	17.70	0.47	0.47
	assign (segid 3A4 and resid 123 and name CB)	(segid 3A4 and resid 135 and name CA)	18.42	0.74	0.74
	assign (segid 3A4 and resid 123 and name CB)	(segid 3A4 and resid 135 and name CB)	17.59	0.92	0.92
15	assign (segid 3A4 and resid 123 and name CB)	(segid 3A4 and resid 147 and name CA)	16.71	1.79	1.79
	assign (segid 3A4 and resid 123 and name CB)	(segid 3A4 and resid 147 and name CB)	17.25	1.72	1.73
	assign (segid 3A4 and resid 123 and name CB)	(segid 3A4 and resid 148 and name CA)	17.35	1.49	1.48
	assign (segid 3A4 and resid 123 and name CB)	(segid 3A4 and resid 149 and name CA)	15.92	1.97	1.97
	assign (segid 3A4 and resid 123 and name CB)	(segid 3A4 and resid 149 and name CB)	16.38	2.63	2.63
20	assign (segid 3A4 and resid 123 and name CB)	(segid 3A4 and resid 150 and name CA)	13.31	1.61	1.61
	assign (segid 3A4 and resid 123 and name CB)	(segid 3A4 and resid 151 and name CA)	13.16	1.79	1.79
	assign (segid 3A4 and resid 123 and name CB)	(segid 3A4 and resid 152 and name CA)	14.81	1.25	1.25
	assign (segid 3A4 and resid 123 and name CB)	(segid 3A4 and resid 152 and name CB)	15.68	1.33	1.32
	assign (segid 3A4 and resid 123 and name CB)	(segid 3A4 and resid 153 and name CA)	14.00	1.47	1.48
25	assign (segid 3A4 and resid 123 and name CB)	(segid 3A4 and resid 153 and name CB)	13.92	2.09	2.08
	assign (segid 3A4 and resid 123 and name CB)	(segid 3A4 and resid 154 and name CA)	12.28	1.48	1.48
	assign (segid 3A4 and resid 123 and name CB)	(segid 3A4 and resid 155 and name CA)	13.81	2.39	2.39
	assign (segid 3A4 and resid 123 and name CB)	(segid 3A4 and resid 155 and name CB)	14.35	2.58	2.58
	assign (segid 3A4 and resid 123 and name CB)	(segid 3A4 and resid 156 and name CA)	15.62	1.33	1.32
30	assign (segid 3A4 and resid 123 and name CB)	(segid 3A4 and resid 156 and name CB)	15.97	1.29	1.28
	assign (segid 3A4 and resid 123 and name CB)	(segid 3A4 and resid 157 and name CA)	14.58	1.29	1.30
	assign (segid 3A4 and resid 123 and name CB)	(segid 3A4 and resid 157 and name CB)	13.90	1.38	1.39
	assign (segid 3A4 and resid 123 and name CB)	(segid 3A4 and resid 160 and name CB)	18.00	1.33	1.34
	assign (segid 3A4 and resid 123 and name CB)	(segid 3A4 and resid 252 and name CA)	18.41	0.81	0.80
35	assign (segid 3A4 and resid 123 and name CB)	(segid 3A4 and resid 252 and name CB)	18.49	0.88	0.88
	assign (segid 3A4 and resid 123 and name CB)	(segid 3A4 and resid 253 and name CA)	17.68	0.46	0.46
	assign (segid 3A4 and resid 123 and name CB)	(segid 3A4 and resid 255 and name CA)	17.43	0.62	0.63
	assign (segid 3A4 and resid 123 and name CB)	(segid 3A4 and resid 256 and name CA)	13.86	0.58	0.57
	assign (segid 3A4 and resid 123 and name CB)	(segid 3A4 and resid 257 and name CA)	13.02	0.68	0.67
40	assign (segid 3A4 and resid 123 and name CB)	(segid 3A4 and resid 258 and name CA)	15.34	0.41	0.42
	assign (segid 3A4 and resid 123 and name CB)	(segid 3A4 and resid 258 and name CB)	16.80	0.43	0.44
	assign (segid 3A4 and resid 123 and name CB)	(segid 3A4 and resid 259 and name CA)	14.37	0.30	0.30
	assign (segid 3A4 and resid 123 and name CB)	(segid 3A4 and resid 259 and name CB)	14.66	0.33	0.33
	assign (segid 3A4 and resid 123 and name CB)	(segid 3A4 and resid 260 and name CA)	10.66	0.30	0.31
45	assign (segid 3A4 and resid 123 and name CB)	(segid 3A4 and resid 260 and name CB)	9.77	0.43	0.43
	assign (segid 3A4 and resid 123 and name CB)	(segid 3A4 and resid 261 and name CA)	11.99	0.52	0.53
	assign (segid 3A4 and resid 123 and name CB)	(segid 3A4 and resid 262 and name CA)	14.66	0.39	0.39
	assign (segid 3A4 and resid 123 and name CB)	(segid 3A4 and resid 262 and name CB)	15.67	0.38	0.37
	assign (segid 3A4 and resid 123 and name CB)	(segid 3A4 and resid 263 and name CA)	12.77	0.25	0.24
50	assign (segid 3A4 and resid 123 and name CB)	(segid 3A4 and resid 263 and name CB)	11.97	0.24	0.25
	assign (segid 3A4 and resid 123 and name CB)	(segid 3A4 and resid 264 and name CA)	10.86	0.31	0.30
	assign (segid 3A4 and resid 123 and name CB)	(segid 3A4 and resid 265 and name CA)	14.34	0.33	0.32
	assign (segid 3A4 and resid 123 and name CB)	(segid 3A4 and resid 266 and name CA)	16.03	0.24	0.24
	assign (segid 3A4 and resid 123 and name CB)	(segid 3A4 and resid 267 and name CA)	14.28	0.26	0.25
55	assign (segid 3A4 and resid 123 and name CB)	(segid 3A4 and resid 267 and name CB)	12.90	0.23	0.22
	assign (segid 3A4 and resid 123 and name CB)	(segid 3A4 and resid 268 and name CA)	15.03	0.40	0.40
	assign (segid 3A4 and resid 123 and name CB)	(segid 3A4 and resid 268 and name CB)	14.73	0.39	0.39
	assign (segid 3A4 and resid 123 and name CB)	(segid 3A4 and resid 269 and name CA)	18.55	0.33	0.33
	assign (segid 3A4 and resid 123 and name CB)	(segid 3A4 and resid 270 and name CA)	19.14	0.38	0.39
60	assign (segid 3A4 and resid 123 and name CB)	(segid 3A4 and resid 270 and name CB)	18.64	0.35	0.35
	assign (segid 3A4 and resid 123 and name CB)	(segid 3A4 and resid 271 and name CA)	18.07	0.55	0.55
	assign (segid 3A4 and resid 123 and name CB)	(segid 3A4 and resid 271 and name CB)	16.75	0.60	0.59
	assign (segid 3A4 and resid 123 and name CB)	(segid 3A4 and resid 318 and name CA)	18.66	1.00	1.00
	assign (segid 3A4 and resid 123 and name CB)	(segid 3A4 and resid 318 and name CB)	17.60	1.02	1.02
65	assign (segid 3A4 and resid 123 and name CB)	(segid 3A4 and resid 400 and name CA)	18.16	0.53	0.54
	assign (segid 3A4 and resid 123 and name CB)	(segid 3A4 and resid 400 and name CB)	17.36	0.55	0.56
	assign (segid 3A4 and resid 123 and name CB)	(segid 3A4 and resid 401 and name CA)	17.71	0.41	0.42
	assign (segid 3A4 and resid 123 and name CB)	(segid 3A4 and resid 404 and name CA)	16.24	0.50	0.51
	assign (segid 3A4 and resid 123 and name CB)	(segid 3A4 and resid 404 and name CB)	15.13	0.48	0.48
70	assign (segid 3A4 and resid 123 and name CB)	(segid 3A4 and resid 405 and name CA)	17.61	0.84	0.83
	assign (segid 3A4 and resid 123 and name CB)	(segid 3A4 and resid 405 and name CB)	18.20	0.82	0.81
	assign (segid 3A4 and resid 123 and name CB)	(segid 3A4 and resid 407 and name CB)	18.42	0.61	0.61
	assign (segid 3A4 and resid 123 and name CB)	(segid 3A4 and resid 408 and name CA)	16.37	0.70	0.71
	assign (segid 3A4 and resid 123 and name CB)	(segid 3A4 and resid 408 and name CB)	15.33	0.66	0.67
75	assign (segid 3A4 and resid 123 and name CB)	(segid 3A4 and resid 411 and name CB)	18.51	0.60	0.59
	assign (segid 3A4 and resid 123 and name CB)	(segid 3A4 and resid 412 and name CA)	18.33	0.55	0.55
	assign (segid 3A4 and resid 123 and name CB)	(segid 3A4 and resid 414 and name CA)	16.86	0.19	0.18
	assign (segid 3A4 and resid 123 and name CB)	(segid 3A4 and resid 415 and name CA)	16.71	0.73	0.73
	assign (segid 3A4 and resid 123 and name CB)	(segid 3A4 and resid 415 and name CB)	17.57	0.84	0.84
80	assign (segid 3A4 and resid 123 and name CB)	(segid 3A4 and resid 416 and name CA)	15.48	0.86	0.86
	assign (segid 3A4 and resid 123 and name CB)	(segid 3A4 and resid 417 and name CA)	16.27	1.49	1.49
	assign (segid 3A4 and resid 123 and name CB)	(segid 3A4 and resid 424 and name CA)	15.64	1.95	1.95
	assign (segid 3A4 and resid 123 and name CB)	(segid 3A4 and resid 426 and name CA)	15.30	1.73	1.72

	assign (segid 3A4 and resid 123 and name CB)	(segid 3A4 and resid 427 and name CA)	15.43	1.67	1.67
	assign (segid 3A4 and resid 123 and name CB)	(segid 3A4 and resid 433 and name CA)	16.67	1.31	1.31
	assign (segid 3A4 and resid 123 and name CB)	(segid 3A4 and resid 434 and name CA)	13.59	1.10	1.10
	assign (segid 3A4 and resid 123 and name CB)	(segid 3A4 and resid 435 and name CA)	11.74	1.24	1.23
	assign (segid 3A4 and resid 123 and name CB)	(segid 3A4 and resid 436 and name CA)	9.90	2.03	2.02
5	assign (segid 3A4 and resid 123 and name CB)	(segid 3A4 and resid 437 and name CA)	8.25	1.67	1.67
	assign (segid 3A4 and resid 123 and name CB)	(segid 3A4 and resid 438 and name CA)	9.35	1.17	1.16
	assign (segid 3A4 and resid 123 and name CB)	(segid 3A4 and resid 439 and name CA)	9.74	0.72	0.72
	assign (segid 3A4 and resid 123 and name CB)	(segid 3A4 and resid 440 and name CA)	11.77	0.39	0.38
	assign (segid 3A4 and resid 123 and name N)	(segid 3A4 and resid 123 and name C)	2.50	0.03	0.03
10	assign (segid 3A4 and resid 123 and name N)	(segid 3A4 and resid 123 and name CB)	1.46	0.00	0.01
	assign (segid 3A4 and resid 123 and name N)	(segid 3A4 and resid 123 and name O)	2.45	0.02	0.03
	assign (segid 3A4 and resid 123 and name N)	(segid 3A4 and resid 124 and name C)	3.52	0.09	0.09
	assign (segid 3A4 and resid 123 and name N)	(segid 3A4 and resid 124 and name CB)	4.86	0.09	0.09
	assign (segid 3A4 and resid 123 and name N)	(segid 3A4 and resid 124 and name O)	4.30	0.07	0.06
15	assign (segid 3A4 and resid 123 and name N)	(segid 3A4 and resid 124 and name CB)	5.13	0.09	0.08
	assign (segid 3A4 and resid 123 and name N)	(segid 3A4 and resid 124 and name N)	2.90	0.09	0.08
	assign (segid 3A4 and resid 123 and name N)	(segid 3A4 and resid 124 and name O)	6.04	0.12	0.12
	assign (segid 3A4 and resid 123 and name N)	(segid 3A4 and resid 125 and name C)	5.67	0.14	0.13
	assign (segid 3A4 and resid 123 and name N)	(segid 3A4 and resid 125 and name CB)	5.52	0.18	0.19
20	assign (segid 3A4 and resid 123 and name N)	(segid 3A4 and resid 125 and name CB)	6.04	0.44	0.44
	assign (segid 3A4 and resid 123 and name N)	(segid 3A4 and resid 125 and name N)	4.41	0.11	0.12
	assign (segid 3A4 and resid 123 and name N)	(segid 3A4 and resid 125 and name O)	6.61	0.15	0.15
	assign (segid 3A4 and resid 123 and name N)	(segid 3A4 and resid 126 and name C)	6.12	0.27	0.27
	assign (segid 3A4 and resid 123 and name N)	(segid 3A4 and resid 126 and name CA)	5.83	0.11	0.11
25	assign (segid 3A4 and resid 123 and name N)	(segid 3A4 and resid 126 and name N)	5.12	0.22	0.21
	assign (segid 3A4 and resid 123 and name N)	(segid 3A4 and resid 126 and name O)	7.25	0.28	0.28
	assign (segid 3A4 and resid 123 and name N)	(segid 3A4 and resid 127 and name CA)	6.20	0.71	0.72
	assign (segid 3A4 and resid 123 and name N)	(segid 3A4 and resid 127 and name CB)	5.63	0.95	0.96
	assign (segid 3A4 and resid 123 and name N)	(segid 3A4 and resid 127 and name N)	5.43	0.50	0.51
30	assign (segid 3A4 and resid 123 and name O)	(segid 3A4 and resid 123 and name CB)	3.25	0.13	0.12
	assign (segid 3A4 and resid 123 and name O)	(segid 3A4 and resid 124 and name C)	3.29	0.21	0.21
	assign (segid 3A4 and resid 123 and name O)	(segid 3A4 and resid 124 and name CA)	2.76	0.04	0.04
	assign (segid 3A4 and resid 123 and name O)	(segid 3A4 and resid 124 and name CB)	4.17	0.06	0.05
35	assign (segid 3A4 and resid 123 and name O)	(segid 3A4 and resid 124 and name N)	2.23	0.01	0.02
	assign (segid 3A4 and resid 123 and name O)	(segid 3A4 and resid 124 and name O)	4.01	0.27	0.26
	assign (segid 3A4 and resid 123 and name O)	(segid 3A4 and resid 125 and name C)	4.95	0.59	0.59
	assign (segid 3A4 and resid 123 and name O)	(segid 3A4 and resid 125 and name CA)	4.75	0.35	0.36
	assign (segid 3A4 and resid 123 and name O)	(segid 3A4 and resid 125 and name CB)	5.90	0.45	0.45
40	assign (segid 3A4 and resid 123 and name O)	(segid 3A4 and resid 125 and name N)	3.63	0.27	0.27
	assign (segid 3A4 and resid 123 and name O)	(segid 3A4 and resid 125 and name O)	5.57	0.34	0.33
	assign (segid 3A4 and resid 123 and name O)	(segid 3A4 and resid 126 and name C)	5.52	1.00	1.00
	assign (segid 3A4 and resid 123 and name O)	(segid 3A4 and resid 126 and name CA)	5.69	1.19	1.19
	assign (segid 3A4 and resid 123 and name O)	(segid 3A4 and resid 126 and name N)	4.88	1.10	1.09
	assign (segid 3A4 and resid 123 and name O)	(segid 3A4 and resid 126 and name O)	6.59	0.96	0.96
45	assign (segid 3A4 and resid 123 and name O)	(segid 3A4 and resid 127 and name C)	5.61	0.39	0.39
	assign (segid 3A4 and resid 123 and name O)	(segid 3A4 and resid 127 and name CA)	4.97	0.53	0.53
	assign (segid 3A4 and resid 123 and name O)	(segid 3A4 and resid 127 and name CB)	4.39	0.27	0.27
	assign (segid 3A4 and resid 123 and name O)	(segid 3A4 and resid 127 and name N)	4.54	0.81	0.81
	assign (segid 3A4 and resid 123 and name O)	(segid 3A4 and resid 127 and name O)	6.74	0.37	0.37
50	assign (segid 3A4 and resid 123 and name O)	(segid 3A4 and resid 128 and name CA)	6.18	0.66	0.67
	assign (segid 3A4 and resid 123 and name O)	(segid 3A4 and resid 128 and name CB)	5.89	0.93	0.92
	assign (segid 3A4 and resid 123 and name O)	(segid 3A4 and resid 128 and name N)	5.20	0.54	0.54
	assign (segid 3A4 and resid 124 and name C)	(segid 3A4 and resid 124 and name CB)	2.47	0.03	0.03
	assign (segid 3A4 and resid 124 and name C)	(segid 3A4 and resid 124 and name O)	1.23	0.01	0.02
55	assign (segid 3A4 and resid 124 and name C)	(segid 3A4 and resid 125 and name C)	3.45	0.24	0.25
	assign (segid 3A4 and resid 124 and name C)	(segid 3A4 and resid 125 and name CA)	2.41	0.02	0.01
	assign (segid 3A4 and resid 124 and name C)	(segid 3A4 and resid 125 and name CB)	3.39	0.19	0.20
	assign (segid 3A4 and resid 124 and name C)	(segid 3A4 and resid 125 and name N)	1.33	0.01	0.01
60	assign (segid 3A4 and resid 124 and name C)	(segid 3A4 and resid 125 and name O)	4.25	0.16	0.15
	assign (segid 3A4 and resid 124 and name C)	(segid 3A4 and resid 126 and name C)	5.52	0.62	0.63
	assign (segid 3A4 and resid 124 and name C)	(segid 3A4 and resid 126 and name CA)	5.27	0.51	0.51
	assign (segid 3A4 and resid 124 and name C)	(segid 3A4 and resid 126 and name N)	3.94	0.45	0.46
	assign (segid 3A4 and resid 124 and name C)	(segid 3A4 and resid 126 and name O)	6.64	0.63	0.62
65	assign (segid 3A4 and resid 124 and name C)	(segid 3A4 and resid 127 and name C)	5.97	0.69	0.68
	assign (segid 3A4 and resid 124 and name C)	(segid 3A4 and resid 127 and name CA)	5.68	0.78	0.78
	assign (segid 3A4 and resid 124 and name C)	(segid 3A4 and resid 127 and name CB)	5.56	0.91	0.90
	assign (segid 3A4 and resid 124 and name C)	(segid 3A4 and resid 127 and name N)	4.87	0.73	0.73
	assign (segid 3A4 and resid 124 and name C)	(segid 3A4 and resid 128 and name C)	6.80	0.46	0.47
70	assign (segid 3A4 and resid 124 and name C)	(segid 3A4 and resid 128 and name CA)	5.90	0.54	0.54
	assign (segid 3A4 and resid 124 and name C)	(segid 3A4 and resid 128 and name CB)	5.21	0.51	0.52
	assign (segid 3A4 and resid 124 and name C)	(segid 3A4 and resid 128 and name N)	5.15	0.62	0.62
	assign (segid 3A4 and resid 124 and name C)	(segid 3A4 and resid 129 and name N)	6.55	0.40	0.40
	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 124 and name C)	1.51	0.01	0.01
75	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 124 and name CB)	1.53	0.01	0.01
	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 124 and name O)	2.37	0.02	0.02
	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 125 and name C)	4.73	0.20	0.20
	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 125 and name CA)	3.80	0.02	0.01
	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 125 and name CB)	4.64	0.17	0.17
	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 125 and name N)	2.45	0.02	0.02
80	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 125 and name O)	5.58	0.12	0.11
	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 126 and name C)	6.38	0.64	0.63
	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 126 and name CA)	6.21	0.51	0.52

	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 126 and name N)	4.97	0.45	0.44
	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 127 and name C)	6.67	0.67	0.66
	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 127 and name CA)	6.18	0.80	0.81
	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 127 and name CB)	5.71	0.96	0.97
	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 127 and name N)	5.53	0.73	0.73
5	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 128 and name CA)	6.82	0.50	0.49
	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 128 and name CB)	6.18	0.51	0.51
	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 128 and name N)	5.98	0.56	0.57
	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 129 and name CA)	8.99	0.36	0.37
	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 129 and name CB)	8.97	0.32	0.32
10	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 130 and name CA)	11.25	0.85	0.84
	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 130 and name CB)	11.17	1.06	1.06
	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 131 and name CA)	11.61	0.74	0.73
	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 131 and name CB)	10.84	0.71	0.72
	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 132 and name CA)	12.57	0.48	0.48
15	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 132 and name CB)	11.95	0.49	0.49
	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 133 and name CA)	14.94	0.50	0.50
	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 133 and name CB)	14.80	0.46	0.46
	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 134 and name CA)	16.38	0.87	0.87
	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 135 and name CA)	16.94	0.58	0.58
20	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 135 and name CB)	16.05	0.50	0.51
	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 136 and name CB)	18.17	0.65	0.64
	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 147 and name CA)	16.31	1.06	1.06
	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 147 and name CB)	16.67	1.18	1.18
	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 148 and name CA)	17.22	1.00	1.00
25	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 149 and name CA)	16.19	1.91	1.91
	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 149 and name CB)	16.54	2.70	2.70
	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 150 and name CA)	13.90	1.31	1.30
	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 151 and name CA)	14.32	1.89	1.89
	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 152 and name CA)	16.18	1.39	1.39
30	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 152 and name CB)	16.85	1.60	1.59
	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 153 and name CA)	15.46	1.71	1.70
	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 153 and name CB)	15.16	2.16	2.16
	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 154 and name CA)	14.22	1.76	1.75
	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 156 and name CA)	17.82	1.58	1.59
35	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 157 and name CA)	16.90	1.60	1.60
	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 157 and name CB)	16.06	1.66	1.66
	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 253 and name CA)	18.54	1.06	1.07
	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 255 and name CA)	17.22	1.18	1.18
	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 256 and name CA)	13.91	1.17	1.18
40	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 257 and name CA)	13.91	1.14	1.15
	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 258 and name CA)	15.69	0.94	0.93
	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 258 and name CB)	17.04	0.97	0.96
	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 259 and name CA)	13.67	0.91	0.90
	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 259 and name CB)	13.65	0.94	0.93
45	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 260 and name CA)	10.36	0.94	0.93
	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 260 and name CB)	9.87	1.13	1.12
	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 261 and name CA)	12.53	0.88	0.88
	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 262 and name CA)	14.22	0.86	0.85
	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 262 and name CB)	15.01	0.91	0.90
50	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 263 and name CA)	11.45	0.74	0.74
	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 263 and name CB)	10.36	0.77	0.76
	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 264 and name CA)	10.53	0.64	0.64
	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 265 and name CA)	14.32	0.63	0.63
	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 266 and name CA)	14.96	0.55	0.54
55	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 267 and name CA)	12.98	0.39	0.40
	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 267 and name CB)	11.51	0.36	0.36
	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 268 and name CA)	14.76	0.49	0.49
	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 268 and name CB)	14.87	0.49	0.48
	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 269 and name CA)	17.96	0.46	0.46
60	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 270 and name CA)	17.76	0.55	0.55
	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 270 and name CB)	16.96	0.50	0.51
	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 271 and name CA)	17.05	0.72	0.73
	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 271 and name CB)	15.91	0.77	0.77
	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 318 and name CB)	18.25	1.07	1.07
65	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 397 and name CA)	18.19	1.01	1.02
	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 400 and name CA)	15.48	0.98	0.99
	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 400 and name CB)	14.90	0.99	1.00
	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 401 and name CA)	15.27	0.86	0.86
	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 402 and name CA)	17.74	0.80	0.80
70	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 403 and name CA)	16.31	0.80	0.80
	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 403 and name CB)	16.29	0.86	0.85
	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 404 and name CA)	12.84	0.78	0.78
	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 404 and name CB)	11.94	0.84	0.84
	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 405 and name CA)	14.51	0.99	0.99
75	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 405 and name CB)	15.35	0.96	0.97
	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 406 and name CA)	17.15	0.85	0.85
	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 407 and name CA)	15.05	0.67	0.68
	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 407 and name CB)	14.43	0.65	0.65
	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 408 and name CA)	12.72	0.65	0.66
80	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 408 and name CB)	11.89	0.61	0.61
	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 409 and name CA)	15.84	0.51	0.51
	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 409 and name CB)	16.68	0.57	0.58

	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 410 and name CA)	17.80	0.53	0.54
	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 411 and name CA)	15.66	0.54	0.55
	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 411 and name CB)	14.53	0.61	0.61
	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 412 and name CA)	14.98	0.56	0.56
	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 413 and name CA)	16.98	0.75	0.75
5	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 414 and name CA)	14.90	0.43	0.43
	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 415 and name CA)	15.70	0.81	0.81
	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 415 and name CB)	16.67	0.76	0.75
	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 416 and name CA)	15.32	0.96	0.96
	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 417 and name CA)	16.59	1.56	1.56
10	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 424 and name CA)	17.44	1.53	1.54
	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 434 and name CA)	15.43	1.14	1.14
	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 435 and name CA)	13.70	0.84	0.84
	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 436 and name CA)	12.83	1.51	1.51
	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 437 and name CA)	11.03	1.42	1.42
15	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 438 and name CA)	10.70	1.23	1.23
	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 439 and name CA)	10.54	0.86	0.86
	assign (segid 3A4 and resid 124 and name CA)	(segid 3A4 and resid 440 and name CA)	11.13	0.72	0.71
	assign (segid 3A4 and resid 124 and name CB)	(segid 3A4 and resid 125 and name C)	5.75	0.18	0.18
	assign (segid 3A4 and resid 124 and name CB)	(segid 3A4 and resid 125 and name CA)	4.58	0.06	0.05
20	assign (segid 3A4 and resid 124 and name CB)	(segid 3A4 and resid 125 and name CB)	5.06	0.25	0.25
	assign (segid 3A4 and resid 124 and name CB)	(segid 3A4 and resid 125 and name N)	3.35	0.07	0.08
	assign (segid 3A4 and resid 124 and name CB)	(segid 3A4 and resid 125 and name O)	6.64	0.16	0.16
	assign (segid 3A4 and resid 124 and name CB)	(segid 3A4 and resid 126 and name CA)	7.34	0.36	0.36
	assign (segid 3A4 and resid 124 and name CB)	(segid 3A4 and resid 126 and name N)	6.01	0.29	0.30
25	assign (segid 3A4 and resid 124 and name CB)	(segid 3A4 and resid 127 and name CA)	7.53	0.91	0.90
	assign (segid 3A4 and resid 124 and name CB)	(segid 3A4 and resid 127 and name CB)	7.01	1.14	1.14
	assign (segid 3A4 and resid 124 and name CB)	(segid 3A4 and resid 127 and name N)	6.86	0.72	0.71
	assign (segid 3A4 and resid 124 and name CB)	(segid 3A4 and resid 128 and name CA)	7.97	0.73	0.74
	assign (segid 3A4 and resid 124 and name CB)	(segid 3A4 and resid 128 and name CB)	7.21	0.66	0.66
30	assign (segid 3A4 and resid 124 and name CB)	(segid 3A4 and resid 129 and name CA)	10.09	0.38	0.38
	assign (segid 3A4 and resid 124 and name CB)	(segid 3A4 and resid 129 and name CB)	9.99	0.31	0.31
	assign (segid 3A4 and resid 124 and name CB)	(segid 3A4 and resid 130 and name CA)	12.51	0.88	0.88
	assign (segid 3A4 and resid 124 and name CB)	(segid 3A4 and resid 130 and name CB)	12.46	1.07	1.07
35	assign (segid 3A4 and resid 124 and name CB)	(segid 3A4 and resid 131 and name CA)	12.86	0.94	0.94
	assign (segid 3A4 and resid 124 and name CB)	(segid 3A4 and resid 131 and name CB)	12.07	0.98	0.98
	assign (segid 3A4 and resid 124 and name CB)	(segid 3A4 and resid 132 and name CA)	13.68	0.58	0.57
	assign (segid 3A4 and resid 124 and name CB)	(segid 3A4 and resid 132 and name CB)	12.99	0.49	0.49
	assign (segid 3A4 and resid 124 and name CB)	(segid 3A4 and resid 133 and name CA)	16.08	0.55	0.56
40	assign (segid 3A4 and resid 124 and name CB)	(segid 3A4 and resid 133 and name CB)	15.96	0.49	0.48
	assign (segid 3A4 and resid 124 and name CB)	(segid 3A4 and resid 134 and name CA)	17.62	1.02	1.02
	assign (segid 3A4 and resid 124 and name CB)	(segid 3A4 and resid 135 and name CA)	18.10	0.78	0.78
	assign (segid 3A4 and resid 124 and name CB)	(segid 3A4 and resid 135 and name CB)	17.17	0.71	0.72
	assign (segid 3A4 and resid 124 and name CB)	(segid 3A4 and resid 147 and name CA)	17.42	1.15	1.14
	assign (segid 3A4 and resid 124 and name CB)	(segid 3A4 and resid 147 and name CB)	17.71	1.20	1.21
45	assign (segid 3A4 and resid 124 and name CB)	(segid 3A4 and resid 149 and name CA)	17.46	1.97	1.97
	assign (segid 3A4 and resid 124 and name CB)	(segid 3A4 and resid 150 and name CA)	15.23	1.39	1.38
	assign (segid 3A4 and resid 124 and name CB)	(segid 3A4 and resid 152 and name CA)	17.54	1.43	1.44
	assign (segid 3A4 and resid 124 and name CB)	(segid 3A4 and resid 153 and name CA)	16.92	1.70	1.71
	assign (segid 3A4 and resid 124 and name CB)	(segid 3A4 and resid 153 and name CB)	16.64	2.17	2.16
50	assign (segid 3A4 and resid 124 and name CB)	(segid 3A4 and resid 154 and name CA)	15.67	1.76	1.76
	assign (segid 3A4 and resid 124 and name CB)	(segid 3A4 and resid 256 and name CA)	15.30	1.23	1.22
	assign (segid 3A4 and resid 124 and name CB)	(segid 3A4 and resid 257 and name CA)	15.24	1.16	1.17
	assign (segid 3A4 and resid 124 and name CB)	(segid 3A4 and resid 258 and name CA)	16.84	0.97	0.97
	assign (segid 3A4 and resid 124 and name CB)	(segid 3A4 and resid 258 and name CB)	18.20	1.00	1.01
55	assign (segid 3A4 and resid 124 and name CB)	(segid 3A4 and resid 259 and name CA)	14.72	1.00	0.99
	assign (segid 3A4 and resid 124 and name CB)	(segid 3A4 and resid 259 and name CB)	14.73	1.05	1.04
	assign (segid 3A4 and resid 124 and name CB)	(segid 3A4 and resid 260 and name CA)	11.44	1.01	1.00
	assign (segid 3A4 and resid 124 and name CB)	(segid 3A4 and resid 260 and name CB)	11.06	1.18	1.17
60	assign (segid 3A4 and resid 124 and name CB)	(segid 3A4 and resid 261 and name CA)	13.43	0.89	0.89
	assign (segid 3A4 and resid 124 and name CB)	(segid 3A4 and resid 262 and name CA)	14.92	0.92	0.93
	assign (segid 3A4 and resid 124 and name CB)	(segid 3A4 and resid 262 and name CB)	15.75	0.99	0.99
	assign (segid 3A4 and resid 124 and name CB)	(segid 3A4 and resid 263 and name CA)	11.95	0.87	0.87
	assign (segid 3A4 and resid 124 and name CB)	(segid 3A4 and resid 263 and name CB)	10.91	0.92	0.91
	assign (segid 3A4 and resid 124 and name CB)	(segid 3A4 and resid 264 and name CA)	10.91	0.69	0.69
65	assign (segid 3A4 and resid 124 and name CB)	(segid 3A4 and resid 265 and name CA)	14.63	0.66	0.67
	assign (segid 3A4 and resid 124 and name CB)	(segid 3A4 and resid 266 and name CA)	15.08	0.62	0.63
	assign (segid 3A4 and resid 124 and name CB)	(segid 3A4 and resid 267 and name CA)	12.79	0.44	0.44
	assign (segid 3A4 and resid 124 and name CB)	(segid 3A4 and resid 267 and name CB)	11.29	0.41	0.41
	assign (segid 3A4 and resid 124 and name CB)	(segid 3A4 and resid 268 and name CA)	14.57	0.50	0.50
70	assign (segid 3A4 and resid 124 and name CB)	(segid 3A4 and resid 268 and name CB)	14.79	0.49	0.49
	assign (segid 3A4 and resid 124 and name CB)	(segid 3A4 and resid 269 and name CA)	17.80	0.48	0.49
	assign (segid 3A4 and resid 124 and name CB)	(segid 3A4 and resid 270 and name CA)	17.37	0.58	0.58
	assign (segid 3A4 and resid 124 and name CB)	(segid 3A4 and resid 270 and name CB)	16.56	0.54	0.55
	assign (segid 3A4 and resid 124 and name CB)	(segid 3A4 and resid 271 and name CA)	16.45	0.74	0.75
75	assign (segid 3A4 and resid 124 and name CB)	(segid 3A4 and resid 271 and name CB)	15.31	0.79	0.80
	assign (segid 3A4 and resid 124 and name CB)	(segid 3A4 and resid 400 and name CA)	16.12	1.16	1.17
	assign (segid 3A4 and resid 124 and name CB)	(segid 3A4 and resid 400 and name CB)	15.66	1.15	1.16
	assign (segid 3A4 and resid 124 and name CB)	(segid 3A4 and resid 401 and name CA)	15.76	1.06	1.06
	assign (segid 3A4 and resid 124 and name CB)	(segid 3A4 and resid 402 and name CA)	17.99	1.01	1.02
80	assign (segid 3A4 and resid 124 and name CB)	(segid 3A4 and resid 403 and name CA)	16.50	1.01	1.00
	assign (segid 3A4 and resid 124 and name CB)	(segid 3A4 and resid 403 and name CB)	16.56	1.04	1.04
	assign (segid 3A4 and resid 124 and name CB)	(segid 3A4 and resid 404 and name CA)	12.95	1.01	1.01

	assign (segid 3A4 and resid 124 and name CB)	(segid 3A4 and resid 404 and name CB)	12.17	1.06	1.06
	assign (segid 3A4 and resid 124 and name CB)	(segid 3A4 and resid 405 and name CA)	14.41	1.18	1.18
	assign (segid 3A4 and resid 124 and name CB)	(segid 3A4 and resid 405 and name CB)	15.32	1.15	1.14
	assign (segid 3A4 and resid 124 and name CB)	(segid 3A4 and resid 406 and name CA)	16.93	1.05	1.04
5	assign (segid 3A4 and resid 124 and name CB)	(segid 3A4 and resid 407 and name CA)	14.69	0.85	0.85
	assign (segid 3A4 and resid 124 and name CB)	(segid 3A4 and resid 407 and name CB)	14.15	0.83	0.82
	assign (segid 3A4 and resid 124 and name CB)	(segid 3A4 and resid 408 and name CA)	12.16	0.80	0.81
	assign (segid 3A4 and resid 124 and name CB)	(segid 3A4 and resid 408 and name CB)	11.40	0.80	0.79
	assign (segid 3A4 and resid 124 and name CB)	(segid 3A4 and resid 409 and name CA)	15.16	0.61	0.62
10	assign (segid 3A4 and resid 124 and name CB)	(segid 3A4 and resid 409 and name CB)	16.08	0.68	0.68
	assign (segid 3A4 and resid 124 and name CB)	(segid 3A4 and resid 410 and name CA)	17.06	0.61	0.61
	assign (segid 3A4 and resid 124 and name CB)	(segid 3A4 and resid 411 and name CA)	14.75	0.50	0.49
	assign (segid 3A4 and resid 124 and name CB)	(segid 3A4 and resid 411 and name CB)	13.65	0.52	0.52
	assign (segid 3A4 and resid 124 and name CB)	(segid 3A4 and resid 412 and name CA)	13.91	0.57	0.57
15	assign (segid 3A4 and resid 124 and name CB)	(segid 3A4 and resid 413 and name CA)	15.83	0.73	0.72
	assign (segid 3A4 and resid 124 and name CB)	(segid 3A4 and resid 414 and name CA)	13.84	0.44	0.44
	assign (segid 3A4 and resid 124 and name CB)	(segid 3A4 and resid 415 and name CA)	14.70	0.76	0.76
	assign (segid 3A4 and resid 124 and name CB)	(segid 3A4 and resid 415 and name CB)	15.63	0.66	0.67
	assign (segid 3A4 and resid 124 and name CB)	(segid 3A4 and resid 416 and name CA)	14.44	0.98	0.99
20	assign (segid 3A4 and resid 124 and name CB)	(segid 3A4 and resid 417 and name CA)	15.62	1.61	1.61
	assign (segid 3A4 and resid 124 and name CB)	(segid 3A4 and resid 434 and name CA)	16.22	1.11	1.11
	assign (segid 3A4 and resid 124 and name CB)	(segid 3A4 and resid 435 and name CA)	14.24	0.85	0.85
	assign (segid 3A4 and resid 124 and name CB)	(segid 3A4 and resid 436 and name CA)	13.41	1.45	1.44
	assign (segid 3A4 and resid 124 and name CB)	(segid 3A4 and resid 437 and name CA)	11.25	1.45	1.45
25	assign (segid 3A4 and resid 124 and name CB)	(segid 3A4 and resid 438 and name CA)	10.52	1.27	1.27
	assign (segid 3A4 and resid 124 and name CB)	(segid 3A4 and resid 439 and name CA)	9.86	0.95	0.95
	assign (segid 3A4 and resid 124 and name CB)	(segid 3A4 and resid 440 and name CA)	10.14	0.78	0.78
	assign (segid 3A4 and resid 124 and name CB)	(segid 3A4 and resid 124 and name C)	2.50	0.02	0.02
	assign (segid 3A4 and resid 124 and name N)	(segid 3A4 and resid 124 and name CA)	1.45	0.00	0.01
30	assign (segid 3A4 and resid 124 and name N)	(segid 3A4 and resid 124 and name CB)	2.46	0.02	0.02
	assign (segid 3A4 and resid 124 and name N)	(segid 3A4 and resid 124 and name O)	3.59	0.03	0.04
	assign (segid 3A4 and resid 124 and name N)	(segid 3A4 and resid 125 and name C)	4.93	0.13	0.13
	assign (segid 3A4 and resid 124 and name N)	(segid 3A4 and resid 125 and name CA)	4.25	0.02	0.02
	assign (segid 3A4 and resid 124 and name N)	(segid 3A4 and resid 125 and name CB)	5.04	0.06	0.07
35	assign (segid 3A4 and resid 124 and name N)	(segid 3A4 and resid 125 and name N)	2.82	0.02	0.02
	assign (segid 3A4 and resid 124 and name N)	(segid 3A4 and resid 125 and name O)	5.86	0.09	0.09
	assign (segid 3A4 and resid 124 and name N)	(segid 3A4 and resid 126 and name C)	6.19	0.36	0.35
	assign (segid 3A4 and resid 124 and name N)	(segid 3A4 and resid 126 and name CA)	6.00	0.38	0.37
40	assign (segid 3A4 and resid 124 and name N)	(segid 3A4 and resid 126 and name N)	4.87	0.37	0.36
	assign (segid 3A4 and resid 124 and name N)	(segid 3A4 and resid 126 and name O)	7.37	0.35	0.36
	assign (segid 3A4 and resid 124 and name N)	(segid 3A4 and resid 127 and name C)	6.76	0.22	0.23
	assign (segid 3A4 and resid 124 and name N)	(segid 3A4 and resid 127 and name CA)	6.04	0.31	0.30
	assign (segid 3A4 and resid 124 and name N)	(segid 3A4 and resid 127 and name CB)	5.48	0.35	0.34
45	assign (segid 3A4 and resid 124 and name N)	(segid 3A4 and resid 127 and name N)	5.33	0.33	0.33
	assign (segid 3A4 and resid 124 and name N)	(segid 3A4 and resid 128 and name CB)	6.83	0.55	0.56
	assign (segid 3A4 and resid 124 and name N)	(segid 3A4 and resid 128 and name N)	6.27	0.30	0.30
	assign (segid 3A4 and resid 124 and name O)	(segid 3A4 and resid 124 and name CB)	3.04	0.08	0.09
50	assign (segid 3A4 and resid 124 and name O)	(segid 3A4 and resid 125 and name C)	3.72	0.40	0.40
	assign (segid 3A4 and resid 124 and name O)	(segid 3A4 and resid 125 and name CA)	2.71	0.03	0.02
	assign (segid 3A4 and resid 124 and name O)	(segid 3A4 and resid 125 and name CB)	3.67	0.31	0.32
	assign (segid 3A4 and resid 124 and name O)	(segid 3A4 and resid 125 and name N)	2.24	0.03	0.02
	assign (segid 3A4 and resid 124 and name O)	(segid 3A4 and resid 125 and name O)	4.27	0.34	0.34
	assign (segid 3A4 and resid 124 and name O)	(segid 3A4 and resid 126 and name C)	5.81	1.03	1.03
	assign (segid 3A4 and resid 124 and name O)	(segid 3A4 and resid 126 and name CA)	5.68	0.79	0.78
55	assign (segid 3A4 and resid 124 and name O)	(segid 3A4 and resid 126 and name N)	4.43	0.64	0.64
	assign (segid 3A4 and resid 124 and name O)	(segid 3A4 and resid 126 and name O)	6.82	1.05	1.04
	assign (segid 3A4 and resid 124 and name O)	(segid 3A4 and resid 127 and name C)	5.90	1.23	1.23
	assign (segid 3A4 and resid 124 and name O)	(segid 3A4 and resid 127 and name CA)	5.86	1.32	1.32
	assign (segid 3A4 and resid 124 and name O)	(segid 3A4 and resid 127 and name CB)	5.85	1.45	1.45
60	assign (segid 3A4 and resid 124 and name O)	(segid 3A4 and resid 127 and name N)	5.18	1.19	1.20
	assign (segid 3A4 and resid 124 and name O)	(segid 3A4 and resid 128 and name CA)	5.49	0.95	0.95
	assign (segid 3A4 and resid 124 and name O)	(segid 3A4 and resid 128 and name CB)	4.69	0.74	0.75
	assign (segid 3A4 and resid 124 and name O)	(segid 3A4 and resid 128 and name N)	4.94	1.14	1.14
	assign (segid 3A4 and resid 124 and name O)	(segid 3A4 and resid 129 and name N)	6.14	0.64	0.63
65	assign (segid 3A4 and resid 125 and name C)	(segid 3A4 and resid 125 and name CB)	2.52	0.02	0.02
	assign (segid 3A4 and resid 125 and name C)	(segid 3A4 and resid 125 and name O)	1.23	0.00	0.00
	assign (segid 3A4 and resid 125 and name C)	(segid 3A4 and resid 126 and name C)	3.05	0.08	0.08
	assign (segid 3A4 and resid 125 and name C)	(segid 3A4 and resid 126 and name CA)	2.43	0.02	0.01
	assign (segid 3A4 and resid 125 and name C)	(segid 3A4 and resid 126 and name N)	1.33	0.01	0.01
70	assign (segid 3A4 and resid 125 and name C)	(segid 3A4 and resid 126 and name O)	3.99	0.13	0.13
	assign (segid 3A4 and resid 125 and name C)	(segid 3A4 and resid 127 and name C)	4.66	0.15	0.14
	assign (segid 3A4 and resid 125 and name C)	(segid 3A4 and resid 127 and name CA)	4.45	0.10	0.10
	assign (segid 3A4 and resid 125 and name C)	(segid 3A4 and resid 127 and name CB)	5.21	0.05	0.06
	assign (segid 3A4 and resid 125 and name C)	(segid 3A4 and resid 127 and name N)	3.22	0.08	0.07
75	assign (segid 3A4 and resid 125 and name C)	(segid 3A4 and resid 127 and name O)	5.66	0.23	0.23
	assign (segid 3A4 and resid 125 and name C)	(segid 3A4 and resid 128 and name C)	5.22	0.23	0.23
	assign (segid 3A4 and resid 125 and name C)	(segid 3A4 and resid 128 and name CA)	4.94	0.19	0.19
	assign (segid 3A4 and resid 125 and name C)	(segid 3A4 and resid 128 and name CB)	4.81	0.22	0.22
	assign (segid 3A4 and resid 125 and name C)	(segid 3A4 and resid 128 and name N)	4.12	0.15	0.11
80	assign (segid 3A4 and resid 125 and name C)	(segid 3A4 and resid 128 and name O)	6.41	0.23	0.23
	assign (segid 3A4 and resid 125 and name C)	(segid 3A4 and resid 129 and name C)	6.10	0.26	0.26
	assign (segid 3A4 and resid 125 and name C)	(segid 3A4 and resid 129 and name CA)	5.30	0.31	0.30
	assign (segid 3A4 and resid 125 and name C)	(segid 3A4 and resid 129 and name CB)	4.81	0.28	0.28

	assign (segid 3A4 and resid 125 and name C)	(segid 3A4 and resid 129 and name N)	4.44	0.26	0.25
	assign (segid 3A4 and resid 125 and name C)	(segid 3A4 and resid 130 and name N)	6.35	0.27	0.27
	assign (segid 3A4 and resid 125 and name C)	(segid 3A4 and resid 260 and name CA)	6.39	1.06	1.06
	assign (segid 3A4 and resid 125 and name C)	(segid 3A4 and resid 260 and name CB)	6.23	1.40	1.40
	assign (segid 3A4 and resid 125 and name C)	(segid 3A4 and resid 260 and name O)	6.60	0.83	0.83
5	assign (segid 3A4 and resid 125 and name C)	(segid 3A4 and resid 263 and name CB)	6.42	0.51	0.52
	assign (segid 3A4 and resid 125 and name CA)	(segid 3A4 and resid 125 and name C)	1.53	0.02	0.01
	assign (segid 3A4 and resid 125 and name CA)	(segid 3A4 and resid 125 and name CB)	1.54	0.00	0.01
	assign (segid 3A4 and resid 125 and name CA)	(segid 3A4 and resid 125 and name O)	2.38	0.03	0.02
	assign (segid 3A4 and resid 125 and name CA)	(segid 3A4 and resid 126 and name C)	4.45	0.04	0.03
10	assign (segid 3A4 and resid 125 and name CA)	(segid 3A4 and resid 126 and name CA)	3.81	0.02	0.03
	assign (segid 3A4 and resid 125 and name CA)	(segid 3A4 and resid 126 and name N)	2.45	0.06	0.05
	assign (segid 3A4 and resid 125 and name CA)	(segid 3A4 and resid 126 and name O)	5.45	0.09	0.09
	assign (segid 3A4 and resid 125 and name CA)	(segid 3A4 and resid 127 and name C)	5.63	0.16	0.15
	assign (segid 3A4 and resid 125 and name CA)	(segid 3A4 and resid 127 and name CA)	5.46	0.05	0.06
15	assign (segid 3A4 and resid 125 and name CA)	(segid 3A4 and resid 127 and name CB)	5.92	0.16	0.17
	assign (segid 3A4 and resid 125 and name CA)	(segid 3A4 and resid 127 and name N)	4.34	0.03	0.04
	assign (segid 3A4 and resid 125 and name CA)	(segid 3A4 and resid 127 and name O)	6.70	0.22	0.22
	assign (segid 3A4 and resid 125 and name CA)	(segid 3A4 and resid 128 and name C)	5.99	0.31	0.31
20	assign (segid 3A4 and resid 125 and name CA)	(segid 3A4 and resid 128 and name CB)	5.52	0.28	0.28
	assign (segid 3A4 and resid 125 and name CA)	(segid 3A4 and resid 128 and name N)	4.99	0.37	0.37
	assign (segid 3A4 and resid 125 and name CA)	(segid 3A4 and resid 128 and name O)	4.85	0.20	0.19
	assign (segid 3A4 and resid 125 and name CA)	(segid 3A4 and resid 129 and name CA)	7.20	0.32	0.31
	assign (segid 3A4 and resid 125 and name CA)	(segid 3A4 and resid 129 and name CB)	6.27	0.42	0.41
25	assign (segid 3A4 and resid 125 and name CA)	(segid 3A4 and resid 129 and name N)	5.81	0.43	0.43
	assign (segid 3A4 and resid 125 and name CA)	(segid 3A4 and resid 130 and name CA)	5.35	0.34	0.34
	assign (segid 3A4 and resid 125 and name CA)	(segid 3A4 and resid 130 and name CB)	8.99	0.31	0.30
	assign (segid 3A4 and resid 125 and name CA)	(segid 3A4 and resid 130 and name N)	9.07	0.32	0.33
30	assign (segid 3A4 and resid 125 and name CA)	(segid 3A4 and resid 131 and name CA)	10.22	0.33	0.33
	assign (segid 3A4 and resid 125 and name CA)	(segid 3A4 and resid 131 and name CB)	9.86	0.29	0.29
	assign (segid 3A4 and resid 125 and name CA)	(segid 3A4 and resid 132 and name CA)	10.85	0.35	0.35
	assign (segid 3A4 and resid 125 and name CA)	(segid 3A4 and resid 132 and name CB)	10.11	0.37	0.37
	assign (segid 3A4 and resid 125 and name CA)	(segid 3A4 and resid 133 and name CA)	12.64	0.45	0.45
	assign (segid 3A4 and resid 125 and name CA)	(segid 3A4 and resid 133 and name CB)	12.28	0.50	0.49
35	assign (segid 3A4 and resid 125 and name CA)	(segid 3A4 and resid 134 and name CA)	14.57	0.33	0.33
	assign (segid 3A4 and resid 125 and name CA)	(segid 3A4 and resid 135 and name CA)	15.56	0.27	0.28
	assign (segid 3A4 and resid 125 and name CA)	(segid 3A4 and resid 135 and name CB)	14.85	0.24	0.24
	assign (segid 3A4 and resid 125 and name CA)	(segid 3A4 and resid 136 and name CA)	16.81	0.48	0.48
	assign (segid 3A4 and resid 125 and name CA)	(segid 3A4 and resid 136 and name CB)	16.16	0.62	0.62
40	assign (segid 3A4 and resid 125 and name CA)	(segid 3A4 and resid 137 and name CA)	18.56	0.51	0.51
	assign (segid 3A4 and resid 125 and name CA)	(segid 3A4 and resid 140 and name CA)	18.99	0.47	0.46
	assign (segid 3A4 and resid 125 and name CA)	(segid 3A4 and resid 140 and name CB)	18.57	0.35	0.35
	assign (segid 3A4 and resid 125 and name CA)	(segid 3A4 and resid 141 and name CA)	17.83	1.49	1.49
	assign (segid 3A4 and resid 125 and name CA)	(segid 3A4 and resid 147 and name CA)	16.69	0.90	0.90
45	assign (segid 3A4 and resid 125 and name CA)	(segid 3A4 and resid 147 and name CB)	17.10	1.50	1.50
	assign (segid 3A4 and resid 125 and name CA)	(segid 3A4 and resid 148 and name CA)	17.84	0.76	0.76
	assign (segid 3A4 and resid 125 and name CA)	(segid 3A4 and resid 149 and name CA)	16.63	1.48	1.48
	assign (segid 3A4 and resid 125 and name CA)	(segid 3A4 and resid 149 and name CB)	16.90	2.16	2.16
	assign (segid 3A4 and resid 125 and name CA)	(segid 3A4 and resid 150 and name CA)	14.33	0.88	0.88
50	assign (segid 3A4 and resid 125 and name CA)	(segid 3A4 and resid 151 and name CA)	15.15	1.71	1.70
	assign (segid 3A4 and resid 125 and name CA)	(segid 3A4 and resid 152 and name CA)	16.73	1.05	1.06
	assign (segid 3A4 and resid 125 and name CA)	(segid 3A4 and resid 152 and name CB)	17.36	1.45	1.44
	assign (segid 3A4 and resid 125 and name CA)	(segid 3A4 and resid 153 and name CA)	15.48	1.47	1.46
	assign (segid 3A4 and resid 125 and name CA)	(segid 3A4 and resid 153 and name CB)	15.08	1.83	1.82
55	assign (segid 3A4 and resid 125 and name CA)	(segid 3A4 and resid 154 and name CA)	14.42	1.66	1.67
	assign (segid 3A4 and resid 125 and name CA)	(segid 3A4 and resid 156 and name CA)	17.74	1.47	1.47
	assign (segid 3A4 and resid 125 and name CA)	(segid 3A4 and resid 157 and name CA)	16.45	1.53	1.54
	assign (segid 3A4 and resid 125 and name CA)	(segid 3A4 and resid 157 and name CB)	15.53	1.62	1.62
	assign (segid 3A4 and resid 125 and name CA)	(segid 3A4 and resid 252 and name CA)	16.82	1.44	1.45
60	assign (segid 3A4 and resid 125 and name CA)	(segid 3A4 and resid 252 and name CB)	17.32	1.48	1.48
	assign (segid 3A4 and resid 125 and name CA)	(segid 3A4 and resid 253 and name CA)	16.89	1.19	1.20
	assign (segid 3A4 and resid 125 and name CA)	(segid 3A4 and resid 254 and name CA)	17.27	1.34	1.34
	assign (segid 3A4 and resid 125 and name CA)	(segid 3A4 and resid 255 and name CA)	14.72	1.31	1.32
	assign (segid 3A4 and resid 125 and name CA)	(segid 3A4 and resid 256 and name CA)	11.78	1.33	1.33
65	assign (segid 3A4 and resid 125 and name CA)	(segid 3A4 and resid 257 and name CA)	11.93	1.49	1.49
	assign (segid 3A4 and resid 125 and name CA)	(segid 3A4 and resid 258 and name CA)	13.05	1.30	1.30
	assign (segid 3A4 and resid 125 and name CA)	(segid 3A4 and resid 258 and name CB)	14.32	1.30	1.30
	assign (segid 3A4 and resid 125 and name CA)	(segid 3A4 and resid 259 and name CA)	10.55	1.16	1.17
	assign (segid 3A4 and resid 125 and name CA)	(segid 3A4 and resid 259 and name CB)	10.49	1.11	1.10
70	assign (segid 3A4 and resid 125 and name CA)	(segid 3A4 and resid 260 and name CA)	7.61	1.36	1.35
	assign (segid 3A4 and resid 125 and name CA)	(segid 3A4 and resid 260 and name CB)	7.52	1.58	1.57
	assign (segid 3A4 and resid 125 and name CA)	(segid 3A4 and resid 261 and name CA)	10.14	1.31	1.32
	assign (segid 3A4 and resid 125 and name CA)	(segid 3A4 and resid 262 and name CA)	11.21	1.22	1.22
	assign (segid 3A4 and resid 125 and name CA)	(segid 3A4 and resid 262 and name CB)	11.83	1.24	1.24
75	assign (segid 3A4 and resid 125 and name CA)	(segid 3A4 and resid 263 and name CA)	8.29	0.97	0.97
	assign (segid 3A4 and resid 125 and name CA)	(segid 3A4 and resid 263 and name CB)	7.06	0.95	0.94
	assign (segid 3A4 and resid 125 and name CA)	(segid 3A4 and resid 264 and name CA)	8.30	0.98	0.99
	assign (segid 3A4 and resid 125 and name CA)	(segid 3A4 and resid 265 and name CA)	12.03	1.02	1.02
	assign (segid 3A4 and resid 125 and name CA)	(segid 3A4 and resid 266 and name CA)	12.24	0.76	0.77
80	assign (segid 3A4 and resid 125 and name CA)	(segid 3A4 and resid 267 and name CA)	10.87	0.47	0.47
	assign (segid 3A4 and resid 125 and name CA)	(segid 3A4 and resid 267 and name CB)	9.52	0.43	0.42
	assign (segid 3A4 and resid 125 and name CA)	(segid 3A4 and resid 268 and name CA)	13.22	0.59	0.59
	assign (segid 3A4 and resid 125 and name CA)	(segid 3A4 and resid 268 and name CB)	13.38	0.67	0.67

assign (segid 3A4 and resid 125 and name CA) (segid 3A4 and resid 269 and name CA) 15.94 0.59 0.59
 assign (segid 3A4 and resid 125 and name CA) (segid 3A4 and resid 270 and name CA) 15.72 0.53 0.53
 assign (segid 3A4 and resid 125 and name CA) (segid 3A4 and resid 270 and name CB) 14.81 0.49 0.49
 assign (segid 3A4 and resid 125 and name CA) (segid 3A4 and resid 271 and name CA) 15.75 0.59 0.59
 assign (segid 3A4 and resid 125 and name CA) (segid 3A4 and resid 271 and name CB) 14.82 0.61 0.61
 5 assign (segid 3A4 and resid 125 and name CA) (segid 3A4 and resid 272 and name CA) 18.66 0.57 0.56
 assign (segid 3A4 and resid 125 and name CA) (segid 3A4 and resid 272 and name CB) 18.68 0.63 0.64
 assign (segid 3A4 and resid 125 and name CA) (segid 3A4 and resid 277 and name CA) 18.48 0.33 0.32
 assign (segid 3A4 and resid 125 and name CA) (segid 3A4 and resid 277 and name CB) 17.87 0.38 0.39
 assign (segid 3A4 and resid 125 and name CA) (segid 3A4 and resid 280 and name CB) 18.37 0.31 0.32
 10 assign (segid 3A4 and resid 125 and name CA) (segid 3A4 and resid 305 and name CA) 18.54 0.75 0.74
 assign (segid 3A4 and resid 125 and name CA) (segid 3A4 and resid 305 and name CB) 17.78 0.78 0.78
 assign (segid 3A4 and resid 125 and name CA) (segid 3A4 and resid 308 and name CB) 18.02 0.75 0.75
 assign (segid 3A4 and resid 125 and name CA) (segid 3A4 and resid 309 and name CA) 16.64 0.89 0.89
 assign (segid 3A4 and resid 125 and name CA) (segid 3A4 and resid 309 and name CB) 16.32 0.97 0.97
 15 assign (segid 3A4 and resid 125 and name CA) (segid 3A4 and resid 312 and name CA) 17.06 0.85 0.86
 assign (segid 3A4 and resid 125 and name CA) (segid 3A4 and resid 312 and name CB) 15.70 0.84 0.85
 assign (segid 3A4 and resid 125 and name CA) (segid 3A4 and resid 313 and name CA) 17.77 0.95 0.95
 assign (segid 3A4 and resid 125 and name CA) (segid 3A4 and resid 313 and name CB) 17.97 0.96 0.96
 assign (segid 3A4 and resid 125 and name CA) (segid 3A4 and resid 316 and name CA) 17.99 1.01 1.01
 20 assign (segid 3A4 and resid 125 and name CA) (segid 3A4 and resid 318 and name CA) 17.00 1.42 1.42
 assign (segid 3A4 and resid 125 and name CA) (segid 3A4 and resid 318 and name CB) 15.68 1.41 1.41
 assign (segid 3A4 and resid 125 and name CA) (segid 3A4 and resid 396 and name CA) 16.88 0.86 0.86
 assign (segid 3A4 and resid 125 and name CA) (segid 3A4 and resid 396 and name CB) 16.89 0.86 0.86
 assign (segid 3A4 and resid 125 and name CA) (segid 3A4 and resid 397 and name CA) 14.74 1.02 1.02
 25 assign (segid 3A4 and resid 125 and name CA) (segid 3A4 and resid 397 and name CB) 15.25 1.13 1.13
 assign (segid 3A4 and resid 125 and name CA) (segid 3A4 and resid 398 and name CA) 16.13 0.90 0.90
 assign (segid 3A4 and resid 125 and name CA) (segid 3A4 and resid 398 and name CB) 17.60 0.91 0.91
 assign (segid 3A4 and resid 125 and name CA) (segid 3A4 and resid 399 and name CA) 15.68 0.76 0.76
 assign (segid 3A4 and resid 125 and name CA) (segid 3A4 and resid 399 and name CB) 16.34 0.80 0.79
 30 assign (segid 3A4 and resid 125 and name CA) (segid 3A4 and resid 400 and name CA) 12.00 0.77 0.77
 assign (segid 3A4 and resid 125 and name CA) (segid 3A4 and resid 400 and name CB) 11.45 0.81 0.81
 assign (segid 3A4 and resid 125 and name CA) (segid 3A4 and resid 401 and name CA) 11.68 0.76 0.75
 assign (segid 3A4 and resid 125 and name CA) (segid 3A4 and resid 402 and name CA) 14.24 0.60 0.61
 35 assign (segid 3A4 and resid 125 and name CA) (segid 3A4 and resid 402 and name CB) 15.64 0.59 0.60
 assign (segid 3A4 and resid 125 and name CA) (segid 3A4 and resid 403 and name CA) 13.04 0.58 0.58
 assign (segid 3A4 and resid 125 and name CA) (segid 3A4 and resid 403 and name CB) 13.04 0.68 0.69
 assign (segid 3A4 and resid 125 and name CA) (segid 3A4 and resid 404 and name CA) 9.64 0.49 0.49
 assign (segid 3A4 and resid 125 and name CA) (segid 3A4 and resid 404 and name CB) 8.63 0.51 0.50
 40 assign (segid 3A4 and resid 125 and name CA) (segid 3A4 and resid 405 and name CA) 11.41 0.74 0.73
 assign (segid 3A4 and resid 125 and name CA) (segid 3A4 and resid 405 and name CB) 12.17 0.79 0.78
 assign (segid 3A4 and resid 125 and name CA) (segid 3A4 and resid 406 and name CA) 14.22 0.58 0.58
 assign (segid 3A4 and resid 125 and name CA) (segid 3A4 and resid 407 and name CA) 12.57 0.66 0.65
 assign (segid 3A4 and resid 125 and name CA) (segid 3A4 and resid 407 and name CB) 11.94 0.73 0.74
 45 assign (segid 3A4 and resid 125 and name CA) (segid 3A4 and resid 408 and name CA) 10.58 0.68 0.67
 assign (segid 3A4 and resid 125 and name CA) (segid 3A4 and resid 408 and name CB) 9.62 0.55 0.55
 assign (segid 3A4 and resid 125 and name CA) (segid 3A4 and resid 409 and name CA) 13.78 0.56 0.56
 assign (segid 3A4 and resid 125 and name CA) (segid 3A4 and resid 409 and name CB) 14.45 0.53 0.53
 assign (segid 3A4 and resid 125 and name CA) (segid 3A4 and resid 410 and name CA) 15.91 0.66 0.66
 50 assign (segid 3A4 and resid 125 and name CA) (segid 3A4 and resid 411 and name CA) 14.42 0.97 0.97
 assign (segid 3A4 and resid 125 and name CA) (segid 3A4 and resid 411 and name CB) 13.31 1.13 1.14
 assign (segid 3A4 and resid 125 and name CA) (segid 3A4 and resid 412 and name CA) 14.08 0.78 0.78
 assign (segid 3A4 and resid 125 and name CA) (segid 3A4 and resid 413 and name CA) 16.44 0.68 0.68
 assign (segid 3A4 and resid 125 and name CA) (segid 3A4 and resid 414 and name CA) 14.43 0.68 0.67
 55 assign (segid 3A4 and resid 125 and name CA) (segid 3A4 and resid 415 and name CA) 15.65 0.83 0.83
 assign (segid 3A4 and resid 125 and name CA) (segid 3A4 and resid 415 and name CB) 16.76 0.79 0.78
 assign (segid 3A4 and resid 125 and name CA) (segid 3A4 and resid 416 and name CA) 15.60 0.87 0.87
 assign (segid 3A4 and resid 125 and name CA) (segid 3A4 and resid 417 and name CA) 17.55 1.47 1.46
 assign (segid 3A4 and resid 125 and name CA) (segid 3A4 and resid 424 and name CA) 17.35 1.16 1.16
 60 assign (segid 3A4 and resid 125 and name CA) (segid 3A4 and resid 425 and name CA) 17.09 0.94 0.94
 assign (segid 3A4 and resid 125 and name CA) (segid 3A4 and resid 426 and name CA) 17.26 0.33 0.33
 assign (segid 3A4 and resid 125 and name CA) (segid 3A4 and resid 427 and name CA) 17.46 0.83 0.83
 assign (segid 3A4 and resid 125 and name CA) (segid 3A4 and resid 433 and name CA) 16.85 1.38 1.38
 assign (segid 3A4 and resid 125 and name CA) (segid 3A4 and resid 434 and name CA) 13.92 1.37 1.37
 65 assign (segid 3A4 and resid 125 and name CA) (segid 3A4 and resid 435 and name CA) 12.73 0.54 0.54
 assign (segid 3A4 and resid 125 and name CA) (segid 3A4 and resid 436 and name CA) 12.76 0.94 0.94
 assign (segid 3A4 and resid 125 and name CA) (segid 3A4 and resid 437 and name CA) 11.68 0.82 0.81
 assign (segid 3A4 and resid 125 and name CA) (segid 3A4 and resid 438 and name CA) 10.97 0.78 0.79
 assign (segid 3A4 and resid 125 and name CA) (segid 3A4 and resid 439 and name CA) 11.67 0.41 0.42
 assign (segid 3A4 and resid 125 and name CA) (segid 3A4 and resid 440 and name CA) 11.79 0.57 0.56
 70 assign (segid 3A4 and resid 125 and name CB) (segid 3A4 and resid 126 and name C) 5.42 0.11 0.12
 assign (segid 3A4 and resid 125 and name CB) (segid 3A4 and resid 126 and name CA) 4.42 0.13 0.13
 assign (segid 3A4 and resid 125 and name CB) (segid 3A4 and resid 126 and name N) 3.11 0.17 0.17
 assign (segid 3A4 and resid 125 and name CB) (segid 3A4 and resid 126 and name O) 6.38 0.16 0.15
 assign (segid 3A4 and resid 125 and name CB) (segid 3A4 and resid 127 and name C) 7.03 0.14 0.14
 75 assign (segid 3A4 and resid 125 and name CB) (segid 3A4 and resid 127 and name CA) 6.80 0.04 0.04
 assign (segid 3A4 and resid 125 and name CB) (segid 3A4 and resid 127 and name CB) 7.31 0.13 0.14
 assign (segid 3A4 and resid 125 and name CB) (segid 3A4 and resid 127 and name N) 5.56 0.08 0.08
 assign (segid 3A4 and resid 125 and name CB) (segid 3A4 and resid 128 and name C) 7.21 0.33 0.34
 80 assign (segid 3A4 and resid 125 and name CB) (segid 3A4 and resid 128 and name CA) 6.91 0.31 0.30
 assign (segid 3A4 and resid 125 and name CB) (segid 3A4 and resid 128 and name CB) 6.32 0.42 0.43
 assign (segid 3A4 and resid 125 and name CB) (segid 3A4 and resid 128 and name N) 6.30 0.19 0.19
 assign (segid 3A4 and resid 125 and name CB) (segid 3A4 and resid 129 and name CA) 7.10 0.45 0.45

	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 129 and name CB)	6.36	0.49	0.48
	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 129 and name N)	6.41	0.36	0.36
	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 130 and name CA)	9.91	0.32	0.32
	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 130 and name CB)	9.98	0.31	0.30
5	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 131 and name CA)	11.48	0.34	0.33
	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 131 and name CB)	11.22	0.28	0.28
	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 132 and name CA)	11.95	0.37	0.37
	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 132 and name CB)	11.13	0.39	0.40
	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 133 and name CA)	13.50	0.51	0.50
10	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 133 and name CB)	13.01	0.56	0.57
	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 134 and name CA)	15.62	0.33	0.33
	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 135 and name CA)	16.74	0.28	0.29
	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 135 and name CB)	16.09	0.23	0.23
	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 136 and name CA)	17.78	0.53	0.53
15	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 136 and name CB)	17.04	0.68	0.67
	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 147 and name CA)	17.94	0.85	0.85
	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 150 and name CA)	15.65	0.85	0.84
	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 151 and name CA)	16.45	1.53	1.52
	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 152 and name CA)	18.02	1.17	1.16
20	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 153 and name CA)	16.69	1.67	1.68
	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 153 and name CB)	16.30	2.04	2.03
	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 154 and name CA)	15.59	1.40	1.40
	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 157 and name CA)	17.39	1.61	1.60
	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 157 and name CB)	16.47	1.66	1.66
25	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 252 and name CA)	17.80	1.68	1.69
	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 253 and name CA)	17.75	1.52	1.53
	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 255 and name CA)	15.36	1.61	1.62
	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 256 and name CA)	12.56	1.62	1.63
	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 257 and name CA)	12.47	1.92	1.92
30	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 258 and name CA)	13.25	1.74	1.74
	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 258 and name CB)	14.52	1.71	1.71
	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 259 and name CA)	10.68	1.51	1.52
	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 259 and name CB)	10.73	1.37	1.38
	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 260 and name CA)	7.80	1.81	1.81
35	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 260 and name CB)	7.94	2.00	2.00
	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 261 and name CA)	9.97	1.84	1.84
	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 262 and name CA)	10.76	1.63	1.64
	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 262 and name CB)	11.44	1.61	1.61
	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 263 and name CA)	7.66	1.26	1.27
40	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 263 and name CB)	6.56	1.19	1.20
	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 264 and name CA)	7.57	1.40	1.39
	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 265 and name CA)	11.23	1.39	1.40
	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 266 and name CA)	11.26	0.96	0.97
	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 267 and name CA)	9.74	0.53	0.54
45	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 267 and name CB)	8.40	0.47	0.48
	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 268 and name CA)	12.16	0.76	0.76
	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 268 and name CB)	12.41	0.91	0.92
	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 269 and name CA)	14.83	0.75	0.75
	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 270 and name CA)	14.49	0.56	0.57
50	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 270 and name CB)	13.58	0.51	0.50
	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 271 and name CA)	14.52	0.62	0.63
	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 271 and name CB)	13.63	0.64	0.64
	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 272 and name CA)	17.46	0.65	0.65
	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 272 and name CB)	17.54	0.77	0.76
55	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 276 and name CB)	19.15	0.54	0.55
	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 277 and name CA)	17.21	0.31	0.31
	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 277 and name CB)	16.59	0.39	0.38
	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 280 and name CA)	18.55	0.24	0.25
	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 280 and name CB)	17.22	0.22	0.21
60	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 281 and name CA)	18.53	0.41	0.42
	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 281 and name CB)	18.45	0.33	0.33
	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 305 and name CA)	17.60	0.79	0.79
	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 305 and name CB)	16.88	0.83	0.82
	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 306 and name CA)	18.86	0.88	0.88
65	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 308 and name CA)	17.78	0.85	0.85
	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 308 and name CB)	16.99	0.80	0.80
	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 309 and name CA)	15.84	1.06	1.07
	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 309 and name CB)	15.59	1.12	1.13
	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 312 and name CA)	16.21	1.12	1.13
70	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 312 and name CB)	14.84	1.09	1.10
	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 313 and name CA)	17.16	1.29	1.29
	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 313 and name CB)	17.43	1.30	1.29
	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 316 and name CA)	17.34	1.39	1.39
	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 318 and name CA)	16.77	1.89	1.89
75	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 318 and name CB)	15.48	1.87	1.87
	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 396 and name CA)	17.08	0.94	0.94
	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 396 and name CB)	17.21	0.95	0.96
	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 397 and name CA)	14.79	1.18	1.19
	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 397 and name CB)	15.28	1.34	1.35
80	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 398 and name CA)	15.88	1.03	1.04
	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 398 and name CB)	17.31	1.05	1.06
	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 399 and name CA)	15.53	0.77	0.77
	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 399 and name CB)	16.29	0.78	0.78

	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 400 and name CA)	11.97	0.75	0.76
	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 400 and name CB)	11.55	0.81	0.82
	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 401 and name CA)	11.27	0.83	0.82
	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 402 and name CA)	13.67	0.60	0.61
5	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 402 and name CB)	15.11	0.61	0.61
	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 403 and name CA)	12.62	0.66	0.67
	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 403 and name CB)	12.79	0.79	0.78
	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 404 and name CA)	9.14	0.58	0.58
	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 404 and name CB)	8.19	0.48	0.49
	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 405 and name CA)	10.52	0.59	0.60
10	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 405 and name CB)	11.26	0.66	0.65
	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 406 and name CA)	13.37	0.59	0.58
	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 407 and name CA)	11.83	0.99	0.99
	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 407 and name CB)	11.34	1.11	1.11
	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 408 and name CA)	9.60	1.03	1.03
15	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 408 and name CB)	8.60	0.84	0.84
	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 409 and name CA)	12.66	0.84	0.84
	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 409 and name CB)	13.30	0.70	0.70
	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 410 and name CA)	14.92	1.03	1.02
	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 411 and name CA)	13.50	1.46	1.47
20	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 411 and name CB)	12.48	1.66	1.67
	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 412 and name CA)	13.01	1.21	1.21
	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 413 and name CA)	15.29	0.89	0.88
	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 414 and name CA)	13.26	0.91	0.91
	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 415 and name CA)	14.58	1.01	1.01
25	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 415 and name CB)	15.72	0.95	0.96
	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 416 and name CA)	14.63	0.93	0.94
	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 417 and name CA)	16.71	1.50	1.50
	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 423 and name CA)	18.10	1.08	1.08
30	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 424 and name CA)	16.70	1.11	1.12
	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 425 and name CA)	16.61	0.71	0.70
	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 426 and name CA)	16.92	0.50	0.50
	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 427 and name CA)	17.29	1.09	1.10
	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 433 and name CA)	16.71	1.86	1.86
35	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 434 and name CA)	13.72	1.81	1.81
	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 435 and name CA)	12.40	0.89	0.89
	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 436 and name CA)	11.50	0.40	0.39
	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 437 and name CA)	10.40	0.49	0.48
40	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 438 and name CA)	11.07	0.28	0.28
	assign (segid 3A4 and resid 125 and name CB)	(segid 3A4 and resid 439 and name CA)	10.90	0.68	0.67
	assign (segid 3A4 and resid 125 and name N)	(segid 3A4 and resid 125 and name C)	2.48	0.04	0.04
	assign (segid 3A4 and resid 125 and name N)	(segid 3A4 and resid 125 and name CA)	1.45	0.00	0.01
	assign (segid 3A4 and resid 125 and name N)	(segid 3A4 and resid 125 and name CB)	2.46	0.03	0.02
45	assign (segid 3A4 and resid 125 and name N)	(segid 3A4 and resid 125 and name O)	3.44	0.07	0.08
	assign (segid 3A4 and resid 125 and name N)	(segid 3A4 and resid 126 and name C)	4.81	0.10	0.10
	assign (segid 3A4 and resid 125 and name N)	(segid 3A4 and resid 126 and name CA)	4.33	0.11	0.12
	assign (segid 3A4 and resid 125 and name N)	(segid 3A4 and resid 126 and name N)	2.93	0.14	0.14
	assign (segid 3A4 and resid 125 and name N)	(segid 3A4 and resid 126 and name O)	5.95	0.09	0.10
50	assign (segid 3A4 and resid 125 and name N)	(segid 3A4 and resid 127 and name C)	5.78	0.15	0.15
	assign (segid 3A4 and resid 125 and name N)	(segid 3A4 and resid 127 and name CA)	5.40	0.13	0.13
	assign (segid 3A4 and resid 125 and name N)	(segid 3A4 and resid 127 and name CB)	5.49	0.25	0.25
	assign (segid 3A4 and resid 125 and name N)	(segid 3A4 and resid 127 and name N)	4.37	0.12	0.12
	assign (segid 3A4 and resid 125 and name N)	(segid 3A4 and resid 127 and name O)	6.96	0.18	0.18
55	assign (segid 3A4 and resid 125 and name N)	(segid 3A4 and resid 128 and name C)	6.66	0.29	0.29
	assign (segid 3A4 and resid 125 and name N)	(segid 3A4 and resid 128 and name CA)	5.89	0.27	0.27
	assign (segid 3A4 and resid 125 and name N)	(segid 3A4 and resid 128 and name CB)	5.34	0.37	0.37
	assign (segid 3A4 and resid 125 and name N)	(segid 3A4 and resid 128 and name N)	5.05	0.20	0.20
	assign (segid 3A4 and resid 125 and name N)	(segid 3A4 and resid 129 and name CA)	7.30	0.37	0.37
60	assign (segid 3A4 and resid 125 and name N)	(segid 3A4 and resid 129 and name CB)	7.02	0.37	0.37
	assign (segid 3A4 and resid 125 and name N)	(segid 3A4 and resid 129 and name N)	6.22	0.32	0.33
	assign (segid 3A4 and resid 125 and name O)	(segid 3A4 and resid 125 and name CB)	3.33	0.15	0.15
	assign (segid 3A4 and resid 125 and name O)	(segid 3A4 and resid 126 and name C)	3.02	0.18	0.19
	assign (segid 3A4 and resid 125 and name O)	(segid 3A4 and resid 126 and name CA)	2.77	0.06	0.05
65	assign (segid 3A4 and resid 125 and name O)	(segid 3A4 and resid 126 and name N)	2.26	0.03	0.02
	assign (segid 3A4 and resid 125 and name O)	(segid 3A4 and resid 126 and name O)	3.66	0.24	0.24
	assign (segid 3A4 and resid 125 and name O)	(segid 3A4 and resid 127 and name C)	4.18	0.36	0.36
	assign (segid 3A4 and resid 125 and name O)	(segid 3A4 and resid 127 and name CA)	4.32	0.33	0.32
	assign (segid 3A4 and resid 125 and name O)	(segid 3A4 and resid 127 and name CB)	5.29	0.29	0.29
70	assign (segid 3A4 and resid 125 and name O)	(segid 3A4 and resid 127 and name N)	3.32	0.26	0.25
	assign (segid 3A4 and resid 125 and name O)	(segid 3A4 and resid 127 and name O)	5.03	0.43	0.42
	assign (segid 3A4 and resid 125 and name O)	(segid 3A4 and resid 128 and name C)	4.24	0.39	0.38
	assign (segid 3A4 and resid 125 and name O)	(segid 3A4 and resid 128 and name CA)	4.18	0.34	0.34
	assign (segid 3A4 and resid 125 and name O)	(segid 3A4 and resid 128 and name CB)	4.15	0.27	0.26
	assign (segid 3A4 and resid 125 and name O)	(segid 3A4 and resid 128 and name N)	3.58	0.36	0.35
75	assign (segid 3A4 and resid 125 and name O)	(segid 3A4 and resid 128 and name O)	5.43	0.39	0.38
	assign (segid 3A4 and resid 125 and name O)	(segid 3A4 and resid 129 and name C)	5.33	0.40	0.40
	assign (segid 3A4 and resid 125 and name O)	(segid 3A4 and resid 129 and name CA)	4.18	0.42	0.42
	assign (segid 3A4 and resid 125 and name O)	(segid 3A4 and resid 129 and name CB)	3.78	0.36	0.35
	assign (segid 3A4 and resid 125 and name O)	(segid 3A4 and resid 129 and name N)	3.35	0.39	0.40
80	assign (segid 3A4 and resid 125 and name O)	(segid 3A4 and resid 129 and name O)	6.44	0.39	0.39
	assign (segid 3A4 and resid 125 and name O)	(segid 3A4 and resid 130 and name CA)	6.78	0.38	0.38
	assign (segid 3A4 and resid 125 and name O)	(segid 3A4 and resid 130 and name CB)	6.94	0.39	0.39

	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 157 and name CA)	13.93	1.61	1.61
	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 157 and name CB)	12.99	1.64	1.63
	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 158 and name CA)	14.35	1.85	1.86
	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 158 and name CB)	14.15	2.19	2.18
5	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 159 and name CA)	17.17	1.38	1.37
	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 159 and name CB)	17.70	1.32	1.33
	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 160 and name CA)	17.68	1.72	1.71
	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 251 and name CA)	16.77	1.51	1.51
	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 251 and name CB)	17.42	1.61	1.60
10	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 252 and name CA)	14.27	1.79	1.78
	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 252 and name CB)	14.84	1.95	1.94
	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 253 and name CA)	13.98	1.43	1.43
	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 254 and name CA)	14.31	1.20	1.19
	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 255 and name CA)	12.02	1.04	1.04
15	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 256 and name CA)	8.96	1.29	1.28
	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 257 and name CA)	8.89	1.18	1.17
	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 258 and name CA)	10.13	0.45	0.45
	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 258 and name CB)	11.40	0.49	0.48
	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 259 and name C)	6.74	0.24	0.24
20	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 259 and name CA)	8.02	0.19	0.18
	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 259 and name CB)	8.08	0.21	0.21
	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 259 and name O)	6.60	0.53	0.52
	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 260 and name C)	5.60	0.28	0.28
	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 260 and name CA)	5.04	0.16	0.16
25	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 260 and name CB)	4.82	0.65	0.65
	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 260 and name N)	6.07	0.18	0.18
	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 261 and name O)	5.31	0.59	0.60
	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 261 and name CA)	7.65	0.26	0.26
	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 261 and name N)	6.73	0.20	0.19
30	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 262 and name CA)	9.12	0.62	0.63
	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 262 and name CB)	9.70	0.56	0.57
	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 263 and name CA)	6.95	1.21	1.20
	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 263 and name CB)	5.76	1.29	1.30
	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 264 and name CA)	7.16	1.04	1.05
35	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 265 and name CA)	10.68	0.93	0.93
	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 266 and name CA)	11.42	1.29	1.29
	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 267 and name CA)	10.90	1.57	1.58
	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 267 and name CB)	9.74	1.63	1.63
	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 268 and name CA)	12.97	1.31	1.31
40	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 268 and name CB)	12.86	1.17	1.17
	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 269 and name CA)	15.51	1.37	1.36
	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 270 and name CA)	15.93	1.52	1.52
	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 270 and name CB)	15.15	1.54	1.54
	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 271 and name CA)	16.34	1.60	1.60
45	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 271 and name CB)	15.42	1.54	1.55
	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 309 and name CA)	15.63	1.06	1.07
	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 309 and name CB)	15.34	0.98	0.98
	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 312 and name CA)	15.66	1.12	1.13
50	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 312 and name CB)	14.42	1.16	1.15
	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 313 and name CA)	15.85	0.79	0.79
	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 313 and name CB)	16.03	0.71	0.71
	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 316 and name CA)	15.97	0.87	0.86
	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 317 and name CA)	16.81	0.69	0.70
	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 318 and name CA)	14.35	0.57	0.57
55	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 318 and name CB)	13.02	0.60	0.61
	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 319 and name CA)	16.79	0.70	0.69
	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 319 and name CB)	16.88	0.73	0.74
	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 383 and name CA)	19.02	0.26	0.26
	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 384 and name CA)	19.16	0.14	0.14
60	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 384 and name CB)	19.14	0.18	0.17
	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 391 and name CB)	18.60	0.42	0.43
	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 393 and name CA)	16.99	0.44	0.44
	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 394 and name CA)	17.38	0.19	0.19
	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 394 and name CB)	18.65	0.25	0.24
65	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 395 and name CA)	18.12	0.25	0.24
	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 396 and name CA)	15.27	0.29	0.29
	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 396 and name CB)	15.18	0.29	0.29
	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 397 and name CA)	12.85	0.24	0.24
	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 397 and name CB)	13.12	0.18	0.19
70	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 398 and name CA)	14.69	0.53	0.53
	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 398 and name CB)	16.14	0.52	0.52
	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 399 and name CA)	14.80	0.67	0.67
	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 399 and name CB)	15.47	0.62	0.61
	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 400 and name CA)	11.16	0.74	0.73
75	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 400 and name CB)	10.33	0.66	0.67
	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 401 and name CA)	10.78	0.88	0.87
	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 402 and name CA)	13.94	1.04	1.03
	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 402 and name CB)	15.26	1.00	1.00
	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 403 and name CA)	13.33	1.13	1.13
80	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 403 and name CB)	13.29	1.08	1.08
	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 404 and name CA)	10.13	1.24	1.24
	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 404 and name CB)	8.78	1.19	1.19
	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 405 and name CA)	11.91	1.18	1.18

	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 405 and name CB)	12.36	1.15	1.16
	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 406 and name CA)	15.14	1.23	1.23
	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 407 and name CA)	14.14	1.39	1.39
	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 407 and name CB)	13.53	1.41	1.40
5	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 408 and name CA)	12.38	1.52	1.52
	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 408 and name CB)	11.22	1.54	1.53
	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 409 and name CA)	15.41	1.58	1.57
	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 409 and name CB)	15.80	1.55	1.56
	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 411 and name CA)	16.87	1.57	1.58
10	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 411 and name CB)	15.84	1.67	1.67
	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 412 and name CA)	16.47	1.43	1.43
	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 414 and name CA)	16.23	1.49	1.48
	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 416 and name CA)	16.77	1.95	1.95
	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 426 and name CA)	15.79	1.15	1.15
15	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 427 and name CA)	15.58	1.08	1.08
	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 428 and name CA)	17.34	1.56	1.55
	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 431 and name CA)	18.05	1.41	1.41
	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 433 and name CA)	14.28	0.78	0.78
	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 434 and name CA)	11.59	0.83	0.83
20	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 435 and name CA)	11.12	1.12	1.12
	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 436 and name CA)	11.53	1.70	1.69
	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 437 and name CA)	11.26	1.55	1.55
	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 438 and name CA)	11.13	1.71	1.70
	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 439 and name CA)	12.80	1.07	1.07
25	assign (segid 3A4 and resid 126 and name CA)	(segid 3A4 and resid 440 and name CA)	13.45	1.35	1.35
	assign (segid 3A4 and resid 126 and name N)	(segid 3A4 and resid 126 and name C)	2.46	0.03	0.03
	assign (segid 3A4 and resid 126 and name N)	(segid 3A4 and resid 126 and name O)	1.46	0.02	0.02
	assign (segid 3A4 and resid 126 and name N)	(segid 3A4 and resid 127 and name C)	3.54	0.02	0.01
	assign (segid 3A4 and resid 126 and name N)	(segid 3A4 and resid 127 and name CA)	4.82	0.10	0.10
30	assign (segid 3A4 and resid 126 and name N)	(segid 3A4 and resid 127 and name CB)	4.23	0.09	0.09
	assign (segid 3A4 and resid 126 and name N)	(segid 3A4 and resid 127 and name N)	5.00	0.14	0.14
	assign (segid 3A4 and resid 126 and name N)	(segid 3A4 and resid 127 and name O)	2.80	0.09	0.09
	assign (segid 3A4 and resid 126 and name N)	(segid 3A4 and resid 128 and name C)	5.82	0.14	0.14
	assign (segid 3A4 and resid 126 and name N)	(segid 3A4 and resid 128 and name CA)	5.95	0.13	0.13
35	assign (segid 3A4 and resid 126 and name N)	(segid 3A4 and resid 128 and name CB)	5.66	0.15	0.16
	assign (segid 3A4 and resid 126 and name N)	(segid 3A4 and resid 128 and name N)	5.78	0.20	0.19
	assign (segid 3A4 and resid 126 and name N)	(segid 3A4 and resid 128 and name O)	4.60	0.13	0.13
	assign (segid 3A4 and resid 126 and name N)	(segid 3A4 and resid 129 and name C)	7.15	0.12	0.13
	assign (segid 3A4 and resid 126 and name N)	(segid 3A4 and resid 129 and name CA)	6.85	0.14	0.14
40	assign (segid 3A4 and resid 126 and name N)	(segid 3A4 and resid 129 and name CB)	5.96	0.12	0.11
	assign (segid 3A4 and resid 126 and name N)	(segid 3A4 and resid 129 and name N)	5.41	0.15	0.14
	assign (segid 3A4 and resid 126 and name N)	(segid 3A4 and resid 130 and name CB)	5.16	0.11	0.11
	assign (segid 3A4 and resid 126 and name N)	(segid 3A4 and resid 130 and name N)	7.53	0.34	0.33
	assign (segid 3A4 and resid 126 and name N)	(segid 3A4 and resid 130 and name O)	6.57	0.23	0.23
45	assign (segid 3A4 and resid 126 and name N)	(segid 3A4 and resid 260 and name C)	6.48	0.44	0.44
	assign (segid 3A4 and resid 126 and name N)	(segid 3A4 and resid 260 and name CA)	6.01	0.57	0.57
	assign (segid 3A4 and resid 126 and name N)	(segid 3A4 and resid 260 and name CB)	5.78	1.07	1.07
	assign (segid 3A4 and resid 126 and name N)	(segid 3A4 and resid 260 and name N)	7.13	0.60	0.59
	assign (segid 3A4 and resid 126 and name N)	(segid 3A4 and resid 260 and name O)	6.05	0.26	0.25
50	assign (segid 3A4 and resid 126 and name N)	(segid 3A4 and resid 263 and name CB)	6.21	0.63	0.64
	assign (segid 3A4 and resid 126 and name N)	(segid 3A4 and resid 264 and name N)	6.97	0.44	0.44
	assign (segid 3A4 and resid 126 and name O)	(segid 3A4 and resid 127 and name C)	3.18	0.12	0.12
	assign (segid 3A4 and resid 126 and name O)	(segid 3A4 and resid 127 and name CA)	2.78	0.04	0.04
	assign (segid 3A4 and resid 126 and name O)	(segid 3A4 and resid 127 and name CB)	4.22	0.04	0.05
55	assign (segid 3A4 and resid 126 and name O)	(segid 3A4 and resid 127 and name N)	2.25	0.01	0.01
	assign (segid 3A4 and resid 126 and name O)	(segid 3A4 and resid 128 and name C)	3.53	0.06	0.06
	assign (segid 3A4 and resid 126 and name O)	(segid 3A4 and resid 128 and name CA)	4.72	0.30	0.30
	assign (segid 3A4 and resid 126 and name O)	(segid 3A4 and resid 128 and name CB)	4.87	0.28	0.28
	assign (segid 3A4 and resid 126 and name O)	(segid 3A4 and resid 128 and name N)	5.85	0.24	0.25
60	assign (segid 3A4 and resid 126 and name O)	(segid 3A4 and resid 128 and name O)	3.85	0.26	0.26
	assign (segid 3A4 and resid 126 and name O)	(segid 3A4 and resid 129 and name C)	5.61	0.31	0.32
	assign (segid 3A4 and resid 126 and name O)	(segid 3A4 and resid 129 and name CA)	4.75	0.40	0.41
	assign (segid 3A4 and resid 126 and name O)	(segid 3A4 and resid 129 and name CB)	4.64	0.27	0.28
	assign (segid 3A4 and resid 126 and name O)	(segid 3A4 and resid 129 and name N)	4.57	0.24	0.23
65	assign (segid 3A4 and resid 126 and name O)	(segid 3A4 and resid 129 and name O)	4.09	0.30	0.29
	assign (segid 3A4 and resid 126 and name O)	(segid 3A4 and resid 130 and name C)	5.94	0.42	0.41
	assign (segid 3A4 and resid 126 and name O)	(segid 3A4 and resid 130 and name CA)	5.71	0.40	0.41
	assign (segid 3A4 and resid 126 and name O)	(segid 3A4 and resid 130 and name CB)	4.78	0.49	0.49
	assign (segid 3A4 and resid 126 and name O)	(segid 3A4 and resid 130 and name N)	4.25	0.44	0.43
70	assign (segid 3A4 and resid 126 and name O)	(segid 3A4 and resid 130 and name O)	3.93	0.46	0.46
	assign (segid 3A4 and resid 126 and name O)	(segid 3A4 and resid 131 and name CA)	6.89	0.41	0.42
	assign (segid 3A4 and resid 126 and name O)	(segid 3A4 and resid 131 and name CB)	6.71	0.32	0.31
	assign (segid 3A4 and resid 126 and name O)	(segid 3A4 and resid 131 and name N)	6.70	0.26	0.26
	assign (segid 3A4 and resid 126 and name O)	(segid 3A4 and resid 131 and name O)	5.49	0.33	0.34
75	assign (segid 3A4 and resid 126 and name O)	(segid 3A4 and resid 256 and name C)	6.77	0.48	0.48
	assign (segid 3A4 and resid 126 and name O)	(segid 3A4 and resid 256 and name CA)	5.95	0.40	0.39
	assign (segid 3A4 and resid 126 and name O)	(segid 3A4 and resid 260 and name C)	5.62	1.15	1.15
	assign (segid 3A4 and resid 126 and name O)	(segid 3A4 and resid 260 and name CA)	4.57	1.05	1.05
	assign (segid 3A4 and resid 126 and name O)	(segid 3A4 and resid 260 and name CB)	4.24	0.57	0.57
80	assign (segid 3A4 and resid 126 and name O)	(segid 3A4 and resid 260 and name N)	5.31	0.87	0.87
	assign (segid 3A4 and resid 127 and name C)	(segid 3A4 and resid 127 and name CB)	2.50	0.04	0.04
	assign (segid 3A4 and resid 127 and name C)	(segid 3A4 and resid 127 and name O)	1.25	0.02	0.01
	assign (segid 3A4 and resid 127 and name C)	(segid 3A4 and resid 128 and name C)	3.09	0.10	0.11

	assign (segid 3A4 and resid 127 and name C) (segid 3A4 and resid 128 and name CA)	2.44	0.02	0.02
	assign (segid 3A4 and resid 127 and name C) (segid 3A4 and resid 128 and name CB)	3.68	0.03	0.02
	assign (segid 3A4 and resid 127 and name C) (segid 3A4 and resid 128 and name N)	1.34	0.01	0.01
	assign (segid 3A4 and resid 127 and name C) (segid 3A4 and resid 128 and name O)	3.93	0.13	0.13
	assign (segid 3A4 and resid 127 and name C) (segid 3A4 and resid 129 and name C)	4.89	0.17	0.18
5	assign (segid 3A4 and resid 127 and name C) (segid 3A4 and resid 129 and name CA)	4.66	0.14	0.15
	assign (segid 3A4 and resid 127 and name C) (segid 3A4 and resid 129 and name CB)	5.42	0.16	0.15
	assign (segid 3A4 and resid 127 and name C) (segid 3A4 and resid 129 and name N)	3.44	0.13	0.13
	assign (segid 3A4 and resid 127 and name C) (segid 3A4 and resid 129 and name O)	5.86	0.14	0.14
10	assign (segid 3A4 and resid 127 and name C) (segid 3A4 and resid 130 and name C)	5.46	0.29	0.29
	assign (segid 3A4 and resid 127 and name C) (segid 3A4 and resid 130 and name CA)	5.31	0.34	0.33
	assign (segid 3A4 and resid 127 and name C) (segid 3A4 and resid 130 and name CB)	5.26	0.40	0.39
	assign (segid 3A4 and resid 127 and name C) (segid 3A4 and resid 130 and name N)	4.45	0.29	0.29
	assign (segid 3A4 and resid 127 and name C) (segid 3A4 and resid 130 and name O)	6.65	0.28	0.29
15	assign (segid 3A4 and resid 127 and name C) (segid 3A4 and resid 131 and name C)	6.24	0.28	0.28
	assign (segid 3A4 and resid 127 and name C) (segid 3A4 and resid 131 and name CA)	5.25	0.28	0.28
	assign (segid 3A4 and resid 127 and name C) (segid 3A4 and resid 131 and name CB)	1.64	0.25	0.25
	assign (segid 3A4 and resid 127 and name C) (segid 3A4 and resid 131 and name N)	4.55	0.28	0.28
	assign (segid 3A4 and resid 127 and name C) (segid 3A4 and resid 132 and name CA)	7.31	0.29	0.28
20	assign (segid 3A4 and resid 127 and name C) (segid 3A4 and resid 132 and name CB)	7.32	0.25	0.25
	assign (segid 3A4 and resid 127 and name C) (segid 3A4 and resid 132 and name N)	6.05	0.30	0.30
	assign (segid 3A4 and resid 127 and name C) (segid 3A4 and resid 256 and name O)	7.30	0.38	0.38
	assign (segid 3A4 and resid 127 and name C) (segid 3A4 and resid 260 and name CB)	6.11	0.71	0.71
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 127 and name C)	1.52	0.01	0.02
25	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 127 and name CB)	1.53	0.01	0.01
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 127 and name O)	2.42	0.03	0.02
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 128 and name C)	4.50	0.10	0.09
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 128 and name CA)	3.81	0.04	0.04
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 128 and name CB)	4.80	0.02	0.03
30	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 128 and name N)	2.44	0.03	0.03
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 128 and name O)	5.40	0.13	0.14
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 129 and name C)	5.96	0.22	0.22
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 129 and name CA)	5.73	0.13	0.13
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 129 and name CB)	6.18	0.14	0.15
35	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 129 and name N)	4.58	0.10	0.10
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 129 and name O)	7.01	0.19	0.20
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 130 and name C)	6.42	0.40	0.41
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 130 and name CA)	6.08	0.45	0.46
40	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 130 and name CB)	5.68	0.55	0.55
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 130 and name N)	5.31	0.36	0.36
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 131 and name CA)	6.42	0.38	0.37
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 131 and name CB)	5.80	0.36	0.36
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 131 and name N)	5.66	0.38	0.37
45	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 132 and name CA)	8.75	0.31	0.32
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 132 and name CB)	8.79	0.26	0.25
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 133 and name CA)	10.60	0.30	0.29
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 133 and name CB)	10.42	0.23	0.22
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 134 and name CA)	11.16	0.52	0.53
50	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 135 and name CA)	12.34	0.39	0.39
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 135 and name CB)	11.74	0.38	0.37
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 136 and name CA)	14.57	0.38	0.39
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 136 and name CB)	14.37	0.43	0.43
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 137 and name CA)	15.86	0.49	0.49
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 138 and name CA)	16.70	0.55	0.56
55	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 138 and name CB)	16.01	0.63	0.64
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 139 and name CA)	17.45	1.08	1.08
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 140 and name CA)	15.48	1.08	1.09
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 140 and name CB)	14.83	0.59	0.59
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 141 and name CA)	14.77	2.49	2.49
60	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 141 and name CB)	15.61	2.91	2.90
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 147 and name CA)	14.02	1.24	1.24
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 147 and name CB)	14.75	1.34	1.33
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 148 and name CA)	14.96	1.51	1.51
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 149 and name CA)	13.07	2.18	2.17
65	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 149 and name CB)	13.18	2.84	2.84
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 150 and name CA)	10.88	1.12	1.13
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 151 and name CA)	11.72	1.43	1.44
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 152 and name CA)	12.91	0.98	0.98
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 152 and name CB)	13.53	1.50	1.49
70	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 153 and name CA)	11.46	1.22	1.22
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 153 and name CB)	11.10	1.56	1.56
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 154 and name CA)	10.42	2.17	2.18
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 155 and name CA)	12.75	2.23	2.22
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 155 and name CB)	13.49	1.96	1.95
75	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 156 and name CA)	13.70	1.39	1.40
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 156 and name CB)	13.71	1.32	1.31
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 157 and name CA)	12.45	2.01	2.01
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 157 and name CB)	11.50	2.11	2.11
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 194 and name CB)	17.27	1.21	1.21
80	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 248 and name CA)	18.68	0.93	0.92
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 249 and name CA)	17.43	0.70	0.70
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 250 and name CA)	17.56	0.25	0.25
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 250 and name CB)	18.86	0.22	0.22

	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 251 and name CA)	15.76	0.42	0.42
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 251 and name CB)	16.32	0.66	0.66
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 252 and name CA)	12.85	0.59	0.58
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 252 and name CB)	13.14	0.78	0.78
5	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 253 and name CA)	12.89	0.24	0.24
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 254 and name CA)	13.92	0.57	0.58
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 255 and name CA)	11.67	0.47	0.47
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 256 and name CA)	8.31	0.27	0.27
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 257 and name CA)	8.85	0.78	0.78
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 258 and name CA)	10.99	0.99	0.98
10	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 258 and name CB)	12.20	0.88	0.88
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 259 and name CA)	9.28	0.92	0.91
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 259 and name CB)	9.08	0.78	0.79
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 260 and name CA)	6.35	1.15	1.14
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 260 and name CB)	5.50	1.00	1.00
15	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 261 and name CA)	9.44	1.20	1.20
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 262 and name CA)	11.48	1.09	1.08
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 262 and name CB)	11.92	1.00	1.01
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 263 and name CA)	9.79	1.05	1.05
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 263 and name CB)	8.57	1.02	1.01
20	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 264 and name CA)	9.96	1.13	1.12
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 265 and name CA)	13.42	1.17	1.18
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 266 and name CA)	14.45	1.08	1.09
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 267 and name CA)	13.96	1.07	1.07
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 267 and name CB)	12.76	1.07	1.06
25	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 268 and name CA)	15.85	1.16	1.15
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 268 and name CB)	15.63	1.20	1.20
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 309 and name CA)	18.30	0.90	0.90
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 309 and name CB)	17.88	0.79	0.80
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 312 and name CB)	17.27	1.25	1.24
30	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 318 and name CA)	15.96	1.33	1.34
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 318 and name CB)	14.63	1.35	1.36
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 393 and name CA)	17.38	0.37	0.37
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 394 and name CA)	18.42	0.49	0.49
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 395 and name CA)	19.13	0.37	0.38
35	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 396 and name CA)	15.92	0.42	0.42
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 396 and name CB)	15.53	0.45	0.44
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 397 and name CA)	14.00	0.40	0.39
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 397 and name CB)	14.32	0.41	0.41
40	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 398 and name CA)	16.39	0.44	0.44
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 398 and name CB)	17.86	0.43	0.43
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 399 and name CA)	16.20	0.48	0.47
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 399 and name CB)	16.59	0.55	0.56
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 400 and name CA)	12.49	0.52	0.53
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 400 and name CB)	11.48	0.59	0.59
45	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 401 and name CA)	12.94	0.45	0.44
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 402 and name CA)	16.13	0.39	0.39
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 402 and name CB)	17.36	0.41	0.40
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 403 and name CA)	15.11	0.42	0.42
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 403 and name CB)	14.78	0.49	0.48
50	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 404 and name CA)	12.21	0.43	0.43
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 404 and name CB)	10.94	0.43	0.43
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 405 and name CA)	14.56	0.61	0.60
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 405 and name CB)	15.11	0.61	0.62
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 406 and name CA)	17.51	0.53	0.52
55	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 407 and name CA)	16.12	0.47	0.46
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 407 and name CB)	15.27	0.46	0.45
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 408 and name CA)	14.67	0.52	0.53
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 408 and name CB)	13.69	0.54	0.53
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 409 and name CA)	17.97	0.55	0.54
60	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 409 and name CB)	18.49	0.60	0.61
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 411 and name CA)	18.76	0.44	0.45
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 411 and name CB)	17.57	0.51	0.51
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 412 and name CA)	18.63	0.38	0.38
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 414 and name CA)	18.70	0.60	0.60
65	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 433 and name CA)	15.56	1.61	1.61
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 434 and name CA)	13.11	1.58	1.58
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 435 and name CA)	12.76	2.19	2.19
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 436 and name CA)	12.36	3.04	3.05
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 437 and name CA)	12.37	2.45	2.45
70	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 438 and name CA)	13.03	2.01	2.00
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 439 and name CA)	14.44	1.09	1.10
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 440 and name CA)	15.47	0.86	0.86
	assign (segid 3A4 and resid 127 and name CA) (segid 3A4 and resid 128 and name C)	5.46	0.11	0.12
	assign (segid 3A4 and resid 127 and name CB) (segid 3A4 and resid 128 and name CA)	4.42	0.06	0.07
75	assign (segid 3A4 and resid 127 and name CB) (segid 3A4 and resid 128 and name CB)	5.20	0.02	0.02
	assign (segid 3A4 and resid 127 and name CB) (segid 3A4 and resid 128 and name N)	3.10	0.07	0.08
	assign (segid 3A4 and resid 127 and name CB) (segid 3A4 and resid 128 and name O)	6.32	0.15	0.16
	assign (segid 3A4 and resid 127 and name CB) (segid 3A4 and resid 129 and name C)	7.31	0.21	0.22
	assign (segid 3A4 and resid 127 and name CB) (segid 3A4 and resid 129 and name CA)	7.02	0.12	0.13
80	assign (segid 3A4 and resid 127 and name CB) (segid 3A4 and resid 129 and name CB)	7.55	0.13	0.13
	assign (segid 3A4 and resid 127 and name CB) (segid 3A4 and resid 129 and name N)	5.76	0.10	0.10
	assign (segid 3A4 and resid 127 and name CB) (segid 3A4 and resid 130 and name CA)	7.45	0.46	0.46

	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 130 and name CB)	7.03	0.57	0.58
	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 130 and name N)	6.74	0.37	0.36
	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 131 and name CA)	7.22	0.42	0.42
	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 131 and name CB)	6.33	0.44	0.43
5	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 131 and name N)	6.70	0.41	0.41
	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 132 and name CA)	9.60	0.38	0.37
	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 132 and name CB)	9.65	0.32	0.31
	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 133 and name CA)	11.76	0.33	0.32
	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 133 and name CB)	11.70	0.24	0.24
10	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 134 and name CA)	12.13	0.58	0.58
	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 135 and name CA)	12.99	0.47	0.48
	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 135 and name CB)	12.28	0.47	0.47
	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 136 and name CA)	15.44	0.46	0.45
	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 136 and name CB)	15.31	0.50	0.50
15	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 137 and name CA)	16.86	0.52	0.51
	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 138 and name CA)	17.45	0.61	0.61
	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 138 and name CB)	16.71	0.74	0.74
	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 139 and name CA)	18.04	1.12	1.12
	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 140 and name CA)	15.83	1.09	1.10
20	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 140 and name CB)	15.17	0.60	0.59
	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 141 and name CA)	14.95	2.54	2.54
	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 141 and name CB)	15.70	2.96	2.95
	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 147 and name CA)	14.05	1.42	1.43
	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 147 and name CB)	14.79	1.49	1.48
25	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 148 and name CA)	14.89	1.47	1.47
	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 149 and name CA)	13.01	1.99	1.98
	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 150 and name CA)	13.15	2.69	2.68
	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 151 and name CA)	10.79	1.31	1.31
	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 151 and name CB)	11.42	1.86	1.87
30	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 152 and name CA)	12.70	1.01	1.02
	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 152 and name CB)	13.36	1.14	1.14
	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 153 and name CA)	11.45	1.10	1.11
	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 153 and name CB)	11.17	1.35	1.34
	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 154 and name CA)	10.23	2.63	2.62
35	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 155 and name CA)	12.40	2.85	2.85
	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 155 and name CB)	13.10	2.59	2.60
	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 156 and name CA)	13.62	1.75	1.75
	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 156 and name CB)	13.70	1.29	1.28
	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 157 and name CA)	12.49	2.38	2.37
40	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 157 and name CB)	11.61	2.41	2.41
	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 194 and name CB)	17.41	1.20	1.20
	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 249 and name CA)	18.03	0.31	0.32
	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 250 and name CA)	18.33	0.22	0.22
	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 251 and name CA)	16.69	0.17	0.18
45	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 251 and name CB)	17.27	0.42	0.41
	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 252 and name CA)	13.65	0.26	0.25
	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 252 and name CB)	13.84	0.41	0.41
	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 253 and name CA)	13.58	0.62	0.62
	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 254 and name CA)	14.85	0.85	0.85
50	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 255 and name CA)	12.74	0.68	0.69
	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 256 and name CA)	9.29	0.60	0.59
	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 257 and name CA)	9.59	1.11	1.11
	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 258 and name CA)	11.95	1.20	1.21
	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 258 and name CB)	13.21	1.10	1.10
55	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 259 and name CA)	10.48	0.94	0.95
	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 259 and name CB)	10.37	0.80	0.80
	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 260 and name CA)	7.36	1.18	1.18
	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 260 and name CB)	6.38	1.14	1.14
	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 261 and name CA)	10.15	1.33	1.34
60	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 262 and name CA)	12.43	1.07	1.06
	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 262 and name CB)	12.97	0.97	0.97
	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 263 and name CA)	10.73	0.88	0.88
	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 263 and name CB)	9.57	0.81	0.81
	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 264 and name CA)	10.49	1.07	1.07
65	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 265 and name CA)	14.00	1.16	1.17
	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 266 and name CA)	15.19	0.93	0.93
	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 267 and name CA)	14.46	0.86	0.85
	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 267 and name CB)	13.20	0.83	0.83
	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 268 and name CA)	16.16	1.07	1.06
70	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 268 and name CB)	15.91	1.16	1.17
	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 312 and name CB)	18.21	1.11	1.12
	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 318 and name CB)	15.44	1.52	1.52
	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 393 and name CA)	18.64	0.42	0.43
	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 396 and name CA)	17.25	0.42	0.42
75	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 396 and name CB)	16.84	0.47	0.46
	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 397 and name CA)	15.33	0.35	0.35
	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 397 and name CB)	15.63	0.38	0.39
	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 398 and name CA)	17.70	0.30	0.30
	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 398 and name CB)	19.17	0.29	0.29
80	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 399 and name CA)	17.49	0.46	0.46
	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 399 and name CB)	17.89	0.59	0.59
	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 400 and name CA)	13.78	0.52	0.52
	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 400 and name CB)	12.80	0.55	0.55

	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 401 and name CA)	14.16	0.26	0.26
	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 402 and name CA)	17.29	0.29	0.30
	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 402 and name CB)	18.54	0.28	0.29
	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 403 and name CA)	16.20	0.53	0.53
5	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 403 and name CB)	15.89	0.59	0.59
	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 404 and name CA)	13.20	0.61	0.60
	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 404 and name CB)	11.97	0.58	0.57
	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 405 and name CA)	15.46	0.78	0.79
	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 405 and name CB)	16.06	0.72	0.71
10	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 406 and name CA)	18.40	0.76	0.75
	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 407 and name CA)	16.85	0.77	0.77
	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 407 and name CB)	16.01	0.78	0.77
	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 408 and name CA)	15.23	0.73	0.74
	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 408 and name CB)	14.26	0.68	0.68
15	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 409 and name CA)	18.52	0.63	0.63
	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 411 and name CB)	17.89	0.77	0.77
	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 414 and name CA)	18.74	0.40	0.41
	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 434 and name CA)	13.42	1.87	1.86
	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 435 and name CA)	12.80	2.44	2.45
20	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 436 and name CA)	12.02	3.39	3.38
	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 437 and name CA)	11.88	2.71	2.71
	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 438 and name CA)	12.75	2.06	2.06
	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 439 and name CA)	13.98	1.07	1.08
	assign (segid 3A4 and resid 127 and name CB)	(segid 3A4 and resid 440 and name CA)	15.19	0.68	0.68
25	assign (segid 3A4 and resid 127 and name N)	(segid 3A4 and resid 127 and name C)	2.49	0.04	0.03
	assign (segid 3A4 and resid 127 and name N)	(segid 3A4 and resid 127 and name CA)	1.46	0.00	0.01
	assign (segid 3A4 and resid 127 and name N)	(segid 3A4 and resid 127 and name CB)	2.46	0.02	0.02
	assign (segid 3A4 and resid 127 and name N)	(segid 3A4 and resid 127 and name O)	3.49	0.07	0.07
	assign (segid 3A4 and resid 127 and name N)	(segid 3A4 and resid 128 and name CA)	4.84	0.09	0.10
30	assign (segid 3A4 and resid 127 and name N)	(segid 3A4 and resid 128 and name CB)	4.30	0.08	0.08
	assign (segid 3A4 and resid 127 and name N)	(segid 3A4 and resid 128 and name N)	5.00	0.05	0.06
	assign (segid 3A4 and resid 127 and name N)	(segid 3A4 and resid 128 and name O)	2.90	0.08	0.08
	assign (segid 3A4 and resid 127 and name N)	(segid 3A4 and resid 129 and name C)	5.92	0.12	0.13
	assign (segid 3A4 and resid 127 and name N)	(segid 3A4 and resid 129 and name CA)	6.08	0.21	0.21
35	assign (segid 3A4 and resid 127 and name N)	(segid 3A4 and resid 129 and name CB)	5.62	0.08	0.09
	assign (segid 3A4 and resid 127 and name N)	(segid 3A4 and resid 129 and name N)	5.72	0.12	0.13
	assign (segid 3A4 and resid 127 and name N)	(segid 3A4 and resid 129 and name O)	4.55	0.07	0.07
	assign (segid 3A4 and resid 127 and name N)	(segid 3A4 and resid 129 and name C)	7.25	0.20	0.19
	assign (segid 3A4 and resid 127 and name N)	(segid 3A4 and resid 130 and name C)	7.09	0.38	0.37
40	assign (segid 3A4 and resid 127 and name N)	(segid 3A4 and resid 130 and name CA)	6.46	0.44	0.44
	assign (segid 3A4 and resid 127 and name N)	(segid 3A4 and resid 130 and name CB)	6.05	0.52	0.51
	assign (segid 3A4 and resid 127 and name N)	(segid 3A4 and resid 130 and name N)	5.50	0.35	0.36
	assign (segid 3A4 and resid 127 and name N)	(segid 3A4 and resid 131 and name CB)	6.99	0.31	0.30
	assign (segid 3A4 and resid 127 and name N)	(segid 3A4 and resid 131 and name N)	6.49	0.33	0.34
45	assign (segid 3A4 and resid 127 and name N)	(segid 3A4 and resid 256 and name O)	7.42	0.14	0.13
	assign (segid 3A4 and resid 127 and name N)	(segid 3A4 and resid 260 and name CA)	5.86	0.74	0.73
	assign (segid 3A4 and resid 127 and name N)	(segid 3A4 and resid 260 and name CB)	5.23	0.44	0.43
	assign (segid 3A4 and resid 127 and name O)	(segid 3A4 and resid 127 and name CB)	3.36	0.05	0.06
	assign (segid 3A4 and resid 127 and name O)	(segid 3A4 and resid 128 and name C)	3.01	0.17	0.17
50	assign (segid 3A4 and resid 127 and name O)	(segid 3A4 and resid 128 and name CA)	2.77	0.02	0.01
	assign (segid 3A4 and resid 127 and name O)	(segid 3A4 and resid 128 and name CB)	4.23	0.02	0.02
	assign (segid 3A4 and resid 127 and name O)	(segid 3A4 and resid 128 and name N)	2.26	0.02	0.01
	assign (segid 3A4 and resid 127 and name O)	(segid 3A4 and resid 128 and name O)	3.49	0.19	0.20
	assign (segid 3A4 and resid 127 and name O)	(segid 3A4 and resid 129 and name C)	4.38	0.29	0.29
55	assign (segid 3A4 and resid 127 and name O)	(segid 3A4 and resid 129 and name CA)	4.51	0.28	0.28
	assign (segid 3A4 and resid 127 and name O)	(segid 3A4 and resid 129 and name CB)	5.47	0.27	0.27
	assign (segid 3A4 and resid 127 and name O)	(segid 3A4 and resid 129 and name N)	3.52	0.23	0.24
	assign (segid 3A4 and resid 127 and name O)	(segid 3A4 and resid 129 and name O)	5.22	0.26	0.27
	assign (segid 3A4 and resid 127 and name O)	(segid 3A4 and resid 130 and name C)	4.40	0.36	0.37
60	assign (segid 3A4 and resid 127 and name O)	(segid 3A4 and resid 130 and name CA)	4.46	0.37	0.37
	assign (segid 3A4 and resid 127 and name O)	(segid 3A4 and resid 130 and name CB)	4.47	0.37	0.37
	assign (segid 3A4 and resid 127 and name O)	(segid 3A4 and resid 130 and name N)	3.84	0.35	0.35
	assign (segid 3A4 and resid 127 and name O)	(segid 3A4 and resid 130 and name O)	5.56	0.35	0.35
	assign (segid 3A4 and resid 127 and name O)	(segid 3A4 and resid 131 and name C)	5.19	0.35	0.34
65	assign (segid 3A4 and resid 127 and name O)	(segid 3A4 and resid 131 and name CA)	4.09	0.32	0.33
	assign (segid 3A4 and resid 127 and name O)	(segid 3A4 and resid 131 and name CB)	3.57	0.25	0.24
	assign (segid 3A4 and resid 127 and name O)	(segid 3A4 and resid 131 and name N)	3.43	0.36	0.36
	assign (segid 3A4 and resid 127 and name O)	(segid 3A4 and resid 131 and name O)	6.33	0.33	0.34
	assign (segid 3A4 and resid 127 and name O)	(segid 3A4 and resid 132 and name CA)	6.50	0.36	0.37
70	assign (segid 3A4 and resid 127 and name O)	(segid 3A4 and resid 132 and name CB)	6.72	0.32	0.33
	assign (segid 3A4 and resid 127 and name O)	(segid 3A4 and resid 132 and name N)	5.16	0.38	0.37
	assign (segid 3A4 and resid 128 and name C)	(segid 3A4 and resid 128 and name CB)	2.50	0.01	0.01
	assign (segid 3A4 and resid 128 and name C)	(segid 3A4 and resid 128 and name O)	1.24	0.01	0.00
	assign (segid 3A4 and resid 128 and name C)	(segid 3A4 and resid 129 and name C)	3.02	0.05	0.06
75	assign (segid 3A4 and resid 128 and name C)	(segid 3A4 and resid 129 and name CA)	2.43	0.00	0.00
	assign (segid 3A4 and resid 128 and name C)	(segid 3A4 and resid 129 and name CB)	3.71	0.03	0.03
	assign (segid 3A4 and resid 128 and name C)	(segid 3A4 and resid 129 and name N)	1.33	0.01	0.01
	assign (segid 3A4 and resid 128 and name C)	(segid 3A4 and resid 129 and name O)	3.71	0.15	0.14
	assign (segid 3A4 and resid 128 and name C)	(segid 3A4 and resid 130 and name C)	4.70	0.05	0.05
80	assign (segid 3A4 and resid 128 and name C)	(segid 3A4 and resid 130 and name CA)	4.67	0.05	0.04
	assign (segid 3A4 and resid 128 and name C)	(segid 3A4 and resid 130 and name CB)	5.47	0.08	0.08
	assign (segid 3A4 and resid 128 and name C)	(segid 3A4 and resid 130 and name N)	3.50	0.06	0.07
	assign (segid 3A4 and resid 128 and name C)	(segid 3A4 and resid 130 and name O)	5.76	0.04	0.05

	assign (segid 3A4 and resid 128 and name C)	(segid 3A4 and resid 131 and name C)	4.88	0.04	0.04
	assign (segid 3A4 and resid 128 and name C)	(segid 3A4 and resid 131 and name CA)	4.63	0.09	0.08
	assign (segid 3A4 and resid 128 and name C)	(segid 3A4 and resid 131 and name CB)	4.49	0.15	0.16
	assign (segid 3A4 and resid 128 and name C)	(segid 3A4 and resid 131 and name N)	3.94	0.07	0.08
5	assign (segid 3A4 and resid 128 and name C)	(segid 3A4 and resid 131 and name O)	6.09	0.04	0.03
	assign (segid 3A4 and resid 128 and name C)	(segid 3A4 and resid 132 and name C)	6.09	0.16	0.16
	assign (segid 3A4 and resid 128 and name C)	(segid 3A4 and resid 132 and name CA)	5.00	0.11	0.10
	assign (segid 3A4 and resid 128 and name C)	(segid 3A4 and resid 132 and name CB)	4.59	0.11	0.12
	assign (segid 3A4 and resid 128 and name C)	(segid 3A4 and resid 132 and name N)	4.10	0.08	0.08
10	assign (segid 3A4 and resid 128 and name C)	(segid 3A4 and resid 132 and name O)	7.25	0.15	0.14
	assign (segid 3A4 and resid 128 and name C)	(segid 3A4 and resid 133 and name CA)	7.28	0.20	0.20
	assign (segid 3A4 and resid 128 and name C)	(segid 3A4 and resid 133 and name CB)	7.36	0.25	0.24
	assign (segid 3A4 and resid 128 and name C)	(segid 3A4 and resid 133 and name CG1)	7.03	0.31	0.32
	assign (segid 3A4 and resid 128 and name C)	(segid 3A4 and resid 133 and name N)	5.99	0.18	0.18
15	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 128 and name C)	1.53	0.02	0.01
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 128 and name CB)	1.54	0.01	0.01
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 128 and name O)	2.39	0.01	0.01
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 129 and name C)	4.47	0.05	0.04
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 129 and name CA)	3.82	0.01	0.02
20	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 129 and name CB)	4.88	0.05	0.05
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 129 and name N)	2.46	0.03	0.03
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 129 and name O)	5.19	0.14	0.15
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 130 and name C)	5.75	0.03	0.04
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 130 and name CA)	5.08	0.08	0.08
25	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 130 and name CB)	6.35	0.16	0.15
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 130 and name N)	4.71	0.09	0.09
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 130 and name O)	6.85	0.04	0.03
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 131 and name C)	5.68	0.10	0.11
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 131 and name CA)	5.25	0.09	0.10
30	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 131 and name CB)	4.67	0.14	0.15
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 131 and name N)	4.78	0.05	0.05
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 131 and name O)	6.86	0.10	0.09
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 132 and name C)	7.24	0.25	0.24
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 132 and name CA)	5.98	0.22	0.23
35	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 132 and name CB)	5.62	0.27	0.28
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 132 and name N)	5.05	0.19	0.19
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 133 and name CA)	8.63	0.24	0.23
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 133 and name CB)	8.79	0.26	0.26
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 133 and name N)	7.28	0.24	0.25
40	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 134 and name CA)	9.98	0.16	0.16
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 135 and name CA)	10.35	0.20	0.21
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 135 and name CB)	9.53	0.21	0.21
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 136 and name CA)	12.10	0.30	0.30
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 136 and name CB)	11.74	0.43	0.44
45	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 137 and name CA)	14.10	0.22	0.21
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 138 and name CA)	15.23	0.21	0.21
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 138 and name CB)	14.77	0.52	0.53
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 139 and name CA)	15.40	0.55	0.55
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 140 and name CA)	13.70	0.36	0.36
50	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 140 and name CB)	13.30	0.39	0.40
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 141 and name CA)	12.73	1.49	1.49
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 141 and name CB)	13.48	2.06	2.06
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 147 and name CA)	12.89	1.94	1.94
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 147 and name CB)	13.48	2.49	2.50
55	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 148 and name CA)	13.94	1.12	1.12
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 149 and name CA)	12.50	0.49	0.49
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 149 and name CB)	12.62	1.00	1.01
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 150 and name CA)	10.61	1.95	1.95
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 151 and name CA)	11.83	2.86	2.86
60	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 152 and name CA)	13.17	1.30	1.30
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 152 and name CB)	13.59	0.83	0.83
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 153 and name CA)	12.05	1.37	1.38
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 153 and name CB)	11.58	1.32	1.33
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 154 and name CA)	11.56	3.29	3.29
65	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 156 and name CA)	14.96	1.79	1.80
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 156 and name CB)	14.72	1.52	1.51
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 157 and name CB)	13.22	2.66	2.67
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 194 and name CA)	18.54	1.00	1.00
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 194 and name CB)	17.99	1.10	1.10
70	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 197 and name CA)	18.16	0.78	0.79
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 219 and name CA)	18.66	0.78	0.78
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 219 and name CB)	17.93	0.74	0.74
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 220 and name CA)	19.03	0.56	0.56
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 220 and name CB)	18.06	0.54	0.53
75	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 248 and name CA)	18.35	0.88	0.88
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 249 and name CA)	17.73	0.75	0.74
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 250 and name CA)	18.03	0.51	0.50
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 251 and name CA)	15.67	0.69	0.69
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 251 and name CB)	15.95	0.89	0.88
80	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 252 and name CA)	12.94	0.65	0.64
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 252 and name CB)	13.25	0.75	0.74
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 253 and name CA)	13.85	0.47	0.47
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 254 and name CA)	14.78	0.45	0.44

	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 255 and name CA)	11.99	0.66	0.66
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 256 and name CA)	9.15	0.40	0.40
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 257 and name CA)	10.75	0.42	0.42
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 258 and name CA)	12.54	0.17	0.17
5	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 258 and name CB)	13.53	0.29	0.28
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 259 and name CA)	10.15	0.40	0.39
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 259 and name CB)	9.50	0.52	0.52
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 260 and name CA)	8.13	0.20	0.20
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 260 and name CB)	7.66	0.31	0.32
10	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 261 and name CA)	11.69	0.18	0.19
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 262 and name CA)	12.95	0.41	0.40
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 262 and name CB)	13.10	0.53	0.52
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 263 and name CA)	10.83	0.49	0.49
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 263 and name CB)	9.38	0.52	0.53
15	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 264 and name CA)	11.85	0.30	0.30
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 265 and name CA)	15.30	0.35	0.36
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 266 and name CA)	15.61	0.50	0.51
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 267 and name CA)	15.10	0.36	0.37
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 267 and name CB)	13.90	0.35	0.35
20	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 268 and name CA)	17.55	0.31	0.32
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 268 and name CB)	17.56	0.30	0.29
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 270 and name CB)	18.99	0.57	0.56
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 309 and name CB)	17.80	1.01	1.02
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 312 and name CB)	18.20	0.76	0.75
25	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 318 and name CA)	17.94	0.81	0.81
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 318 and name CB)	16.53	0.81	0.81
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 393 and name CA)	16.98	0.79	0.78
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 394 and name CA)	18.16	0.76	0.76
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 395 and name CA)	18.25	0.87	0.88
30	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 396 and name CA)	14.78	0.86	0.86
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 396 and name CB)	14.37	0.82	0.82
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 397 and name CA)	13.51	0.89	0.88
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 397 and name CB)	14.15	0.86	0.87
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 398 and name CA)	15.77	0.95	0.95
35	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 398 and name CB)	17.25	0.94	0.95
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 399 and name CA)	14.84	1.05	1.05
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 399 and name CB)	15.05	1.10	1.10
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 400 and name CA)	11.13	1.05	1.06
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 400 and name CB)	10.22	0.95	0.96
40	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 401 and name CA)	12.33	1.02	1.03
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 402 and name CA)	15.12	1.06	1.07
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 402 and name CB)	16.27	1.04	1.03
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 403 and name CA)	13.45	1.08	1.07
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 403 and name CB)	12.89	1.05	1.04
45	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 404 and name CA)	10.92	1.20	1.20
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 404 and name CB)	9.88	1.29	1.28
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 405 and name CA)	13.87	1.36	1.37
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 405 and name CB)	14.64	1.34	1.34
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 406 and name CA)	16.29	1.21	1.21
50	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 407 and name CA)	14.55	1.01	1.01
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 407 and name CB)	13.49	0.96	0.95
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 408 and name CA)	13.73	0.90	0.91
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 408 and name CB)	13.03	0.88	0.88
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 409 and name CA)	17.29	0.89	0.89
55	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 409 and name CB)	17.93	0.97	0.96
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 411 and name CA)	17.55	0.79	0.78
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 411 and name CB)	16.26	0.75	0.74
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 412 and name CA)	18.04	0.86	0.86
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 433 and name CA)	18.15	0.98	0.98
60	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 434 and name CA)	15.87	0.89	0.88
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 435 and name CA)	15.52	1.15	1.14
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 437 and name CA)	15.08	1.84	1.84
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 438 and name CA)	15.32	1.37	1.37
	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 439 and name CA)	16.31	0.72	0.72
65	assign (segid 3A4 and resid 128 and name CA)	(segid 3A4 and resid 440 and name CA)	16.77	0.44	0.44
	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 129 and name C)	5.42	0.06	0.05
	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 129 and name CA)	4.43	0.03	0.04
	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 129 and name CB)	5.29	0.09	0.09
	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 129 and name N)	3.12	0.04	0.05
70	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 129 and name O)	6.08	0.18	0.18
	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 130 and name C)	7.11	0.04	0.04
	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 130 and name CA)	7.09	0.07	0.07
	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 130 and name CB)	7.71	0.14	0.15
	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 130 and name N)	5.88	0.08	0.09
75	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 131 and name C)	6.83	0.14	0.13
	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 131 and name CA)	6.60	0.12	0.13
	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 131 and name CB)	6.00	0.19	0.20
	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 131 and name N)	6.19	0.08	0.08
	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 132 and name CA)	6.69	0.24	0.23
80	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 132 and name CB)	6.03	0.31	0.30
	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 132 and name N)	6.02	0.19	0.19
	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 133 and name CA)	9.50	0.27	0.27
	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 133 and name CB)	9.70	0.29	0.30

	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 134 and name CA)	11.18	0.13	0.12
	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 135 and name CA)	11.28	0.25	0.24
	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 135 and name CB)	10.35	0.28	0.28
	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 136 and name CA)	12.77	0.31	0.32
5	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 136 and name CB)	12.31	0.43	0.44
	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 137 and name CA)	15.02	0.21	0.22
	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 138 and name CA)	16.26	0.22	0.23
	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 138 and name CB)	15.87	0.57	0.57
	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 139 and name CA)	16.20	0.38	0.39
10	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 140 and name CA)	14.51	0.28	0.27
	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 140 and name CB)	14.20	0.63	0.63
	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 141 and name CA)	13.30	1.13	1.12
	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 141 and name CB)	13.98	1.73	1.72
	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 147 and name CA)	13.31	2.42	2.42
15	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 147 and name CB)	13.79	3.02	3.03
	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 148 and name CA)	14.32	1.67	1.67
	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 149 and name CA)	13.13	0.61	0.60
	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 149 and name CB)	13.32	0.68	0.69
	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 150 and name CA)	11.26	2.32	2.31
20	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 151 and name CA)	12.38	3.31	3.30
	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 152 and name CA)	13.88	1.62	1.62
	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 152 and name CB)	14.29	0.99	0.99
	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 153 and name CA)	12.97	1.51	1.52
	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 153 and name CB)	12.52	1.43	1.44
25	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 154 and name CA)	12.49	3.40	3.41
	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 156 and name CA)	15.91	1.85	1.85
	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 156 and name CB)	15.67	1.56	1.57
	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 219 and name CB)	18.72	0.67	0.67
	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 220 and name CB)	19.05	0.59	0.59
30	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 251 and name CA)	16.90	0.91	0.90
	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 251 and name CB)	17.15	1.08	1.08
	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 252 and name CA)	14.21	0.78	0.77
	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 252 and name CB)	14.52	0.84	0.83
	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 253 and name CA)	15.12	0.52	0.52
35	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 254 and name CA)	15.98	0.63	0.63
	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 255 and name CA)	13.15	0.90	0.91
	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 256 and name CA)	10.38	0.64	0.63
	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 257 and name CA)	11.82	0.59	0.60
	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 258 and name CA)	13.47	0.69	0.70
40	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 258 and name CB)	14.49	0.79	0.79
	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 259 and name CA)	10.93	1.00	0.99
	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 259 and name CB)	10.32	1.08	1.07
	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 260 and name CA)	8.82	0.77	0.76
	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 260 and name CB)	8.46	0.74	0.74
45	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 261 and name CA)	12.28	0.69	0.68
	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 262 and name CA)	13.37	1.10	1.11
	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 262 and name CB)	13.57	1.23	1.23
	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 263 and name CA)	10.96	1.19	1.18
	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 263 and name CB)	9.49	1.22	1.22
50	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 264 and name CA)	11.92	0.84	0.85
	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 265 and name CA)	15.44	0.96	0.97
	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 266 and name CA)	15.58	1.18	1.18
	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 267 and name CA)	14.83	0.95	0.94
	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 267 and name CB)	13.58	0.86	0.86
55	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 268 and name CA)	17.36	0.82	0.81
	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 268 and name CB)	17.45	0.78	0.78
	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 318 and name CB)	17.23	1.10	1.10
	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 393 and name CA)	17.91	1.23	1.23
	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 396 and name CA)	15.45	1.34	1.33
60	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 396 and name CB)	15.13	1.25	1.25
	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 397 and name CA)	14.16	1.46	1.47
	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 397 and name CB)	14.87	1.45	1.45
	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 398 and name CA)	16.18	1.60	1.59
	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 398 and name CB)	17.67	1.59	1.59
65	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 399 and name CA)	15.11	1.62	1.62
	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 399 and name CB)	15.37	1.61	1.61
	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 400 and name CA)	11.38	1.63	1.64
	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 400 and name CB)	10.61	1.51	1.51
	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 401 and name CA)	12.46	1.71	1.70
70	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 402 and name CA)	15.06	1.72	1.72
	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 402 and name CB)	16.25	1.67	1.68
	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 403 and name CA)	13.23	1.61	1.62
	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 403 and name CB)	12.73	1.54	1.54
	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 404 and name CA)	10.57	1.79	1.79
75	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 404 and name CB)	9.61	1.92	1.91
	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 405 and name CA)	13.48	1.97	1.97
	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 405 and name CB)	14.34	1.98	1.97
	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 406 and name CA)	15.80	1.75	1.75
	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 407 and name CA)	13.88	1.42	1.42
80	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 407 and name CB)	12.83	1.33	1.33
	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 408 and name CA)	12.99	1.33	1.32
	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 408 and name CB)	12.34	1.33	1.34
	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 409 and name CA)	16.57	1.34	1.33

	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 409 and name CB)	17.27	1.45	1.45
	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 411 and name CA)	16.62	1.04	1.04
	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 411 and name CB)	15.33	0.95	0.95
	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 412 and name CA)	17.13	1.16	1.16
5	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 434 and name CA)	16.41	0.90	0.91
	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 435 and name CA)	15.80	0.76	0.76
	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 436 and name CA)	15.50	1.86	1.86
	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 437 and name CA)	15.05	1.59	1.59
	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 438 and name CA)	15.09	1.15	1.15
10	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 439 and name CA)	15.82	0.67	0.68
	assign (segid 3A4 and resid 128 and name CB)	(segid 3A4 and resid 440 and name CA)	16.11	0.48	0.48
	assign (segid 3A4 and resid 128 and name N)	(segid 3A4 and resid 128 and name C)	2.50	0.02	0.02
	assign (segid 3A4 and resid 128 and name N)	(segid 3A4 and resid 128 and name CA)	1.46	0.01	0.01
	assign (segid 3A4 and resid 128 and name N)	(segid 3A4 and resid 128 and name CB)	2.41	0.05	0.04
15	assign (segid 3A4 and resid 128 and name N)	(segid 3A4 and resid 128 and name O)	3.53	0.04	0.03
	assign (segid 3A4 and resid 128 and name N)	(segid 3A4 and resid 129 and name C)	4.92	0.04	0.05
	assign (segid 3A4 and resid 128 and name N)	(segid 3A4 and resid 129 and name CA)	4.33	0.04	0.04
	assign (segid 3A4 and resid 128 and name N)	(segid 3A4 and resid 129 and name CB)	5.09	0.10	0.11
	assign (segid 3A4 and resid 128 and name N)	(segid 3A4 and resid 129 and name O)	2.92	0.05	0.04
20	assign (segid 3A4 and resid 128 and name N)	(segid 3A4 and resid 130 and name C)	5.86	0.05	0.06
	assign (segid 3A4 and resid 128 and name N)	(segid 3A4 and resid 130 and name CA)	6.06	0.13	0.13
	assign (segid 3A4 and resid 128 and name N)	(segid 3A4 and resid 130 and name CB)	5.91	0.20	0.19
	assign (segid 3A4 and resid 128 and name N)	(segid 3A4 and resid 130 and name O)	6.11	0.27	0.28
	assign (segid 3A4 and resid 128 and name N)	(segid 3A4 and resid 130 and name N)	4.82	0.17	0.18
25	assign (segid 3A4 and resid 128 and name N)	(segid 3A4 and resid 131 and name C)	7.25	0.13	0.12
	assign (segid 3A4 and resid 128 and name N)	(segid 3A4 and resid 131 and name CA)	6.50	0.14	0.15
	assign (segid 3A4 and resid 128 and name N)	(segid 3A4 and resid 131 and name CB)	5.78	0.15	0.14
	assign (segid 3A4 and resid 128 and name N)	(segid 3A4 and resid 131 and name O)	5.15	0.15	0.14
	assign (segid 3A4 and resid 128 and name N)	(segid 3A4 and resid 131 and name N)	5.14	0.11	0.11
30	assign (segid 3A4 and resid 128 and name N)	(segid 3A4 and resid 132 and name C)	7.70	0.15	0.14
	assign (segid 3A4 and resid 128 and name N)	(segid 3A4 and resid 132 and name CA)	7.15	0.21	0.21
	assign (segid 3A4 and resid 128 and name N)	(segid 3A4 and resid 132 and name CB)	6.91	0.23	0.22
	assign (segid 3A4 and resid 128 and name N)	(segid 3A4 and resid 132 and name O)	6.06	0.20	0.20
	assign (segid 3A4 and resid 128 and name N)	(segid 3A4 and resid 132 and name N)	7.37	0.18	0.18
35	assign (segid 3A4 and resid 128 and name N)	(segid 3A4 and resid 133 and name C)	6.79	0.24	0.24
	assign (segid 3A4 and resid 128 and name N)	(segid 3A4 and resid 133 and name CA)	3.31	0.05	0.05
	assign (segid 3A4 and resid 128 and name N)	(segid 3A4 and resid 133 and name CB)	2.90	0.09	0.10
	assign (segid 3A4 and resid 128 and name N)	(segid 3A4 and resid 133 and name O)	2.75	0.03	0.03
	assign (segid 3A4 and resid 128 and name N)	(segid 3A4 and resid 133 and name N)	4.24	0.04	0.04
40	assign (segid 3A4 and resid 128 and name N)	(segid 3A4 and resid 134 and name C)	2.25	0.01	0.01
	assign (segid 3A4 and resid 128 and name N)	(segid 3A4 and resid 134 and name CA)	3.18	0.20	0.20
	assign (segid 3A4 and resid 128 and name N)	(segid 3A4 and resid 134 and name CB)	4.16	0.11	0.12
	assign (segid 3A4 and resid 128 and name N)	(segid 3A4 and resid 134 and name O)	4.45	0.12	0.11
	assign (segid 3A4 and resid 128 and name N)	(segid 3A4 and resid 134 and name N)	5.47	0.13	0.13
45	assign (segid 3A4 and resid 128 and name N)	(segid 3A4 and resid 135 and name C)	3.54	0.10	0.10
	assign (segid 3A4 and resid 128 and name N)	(segid 3A4 and resid 135 and name CA)	5.07	0.09	0.08
	assign (segid 3A4 and resid 128 and name N)	(segid 3A4 and resid 135 and name CB)	3.82	0.08	0.08
	assign (segid 3A4 and resid 128 and name N)	(segid 3A4 and resid 135 and name O)	3.84	0.16	0.15
	assign (segid 3A4 and resid 128 and name N)	(segid 3A4 and resid 135 and name N)	3.86	0.26	0.27
50	assign (segid 3A4 and resid 128 and name N)	(segid 3A4 and resid 136 and name C)	3.37	0.17	0.17
	assign (segid 3A4 and resid 128 and name N)	(segid 3A4 and resid 136 and name CA)	4.99	0.07	0.07
	assign (segid 3A4 and resid 128 and name N)	(segid 3A4 and resid 136 and name CB)	4.92	0.18	0.19
	assign (segid 3A4 and resid 128 and name N)	(segid 3A4 and resid 136 and name O)	3.79	0.11	0.12
	assign (segid 3A4 and resid 128 and name N)	(segid 3A4 and resid 136 and name N)	3.50	0.18	0.18
55	assign (segid 3A4 and resid 128 and name N)	(segid 3A4 and resid 137 and name C)	2.94	0.06	0.06
	assign (segid 3A4 and resid 128 and name N)	(segid 3A4 and resid 137 and name CA)	6.06	0.17	0.17
	assign (segid 3A4 and resid 128 and name N)	(segid 3A4 and resid 137 and name CB)	7.14	0.14	0.14
	assign (segid 3A4 and resid 128 and name N)	(segid 3A4 and resid 137 and name O)	6.29	0.24	0.24
	assign (segid 3A4 and resid 128 and name N)	(segid 3A4 and resid 137 and name N)	6.55	0.30	0.30
60	assign (segid 3A4 and resid 128 and name N)	(segid 3A4 and resid 138 and name C)	6.33	0.35	0.35
	assign (segid 3A4 and resid 128 and name N)	(segid 3A4 and resid 138 and name CA)	4.93	0.23	0.23
	assign (segid 3A4 and resid 128 and name N)	(segid 3A4 and resid 138 and name CB)	6.84	0.11	0.11
	assign (segid 3A4 and resid 128 and name N)	(segid 3A4 and resid 138 and name O)	7.66	0.13	0.12
	assign (segid 3A4 and resid 128 and name N)	(segid 3A4 and resid 138 and name N)	2.56	0.02	0.02
65	assign (segid 3A4 and resid 129 and name C)	(segid 3A4 and resid 129 and name O)	1.23	0.00	0.01
	assign (segid 3A4 and resid 129 and name C)	(segid 3A4 and resid 130 and name C)	3.07	0.05	0.05
	assign (segid 3A4 and resid 129 and name C)	(segid 3A4 and resid 130 and name CA)	2.44	0.02	0.03
	assign (segid 3A4 and resid 129 and name C)	(segid 3A4 and resid 130 and name CB)	3.66	0.04	0.04
	assign (segid 3A4 and resid 129 and name C)	(segid 3A4 and resid 130 and name O)	1.34	0.01	0.01
70	assign (segid 3A4 and resid 129 and name C)	(segid 3A4 and resid 130 and name N)	3.98	0.09	0.08
	assign (segid 3A4 and resid 129 and name C)	(segid 3A4 and resid 131 and name C)	4.62	0.11	0.11
	assign (segid 3A4 and resid 129 and name C)	(segid 3A4 and resid 131 and name CA)	4.48	0.07	0.06
	assign (segid 3A4 and resid 129 and name C)	(segid 3A4 and resid 131 and name CB)	5.26	0.10	0.11
	assign (segid 3A4 and resid 129 and name C)	(segid 3A4 and resid 131 and name O)	3.27	0.05	0.06
75	assign (segid 3A4 and resid 129 and name C)	(segid 3A4 and resid 131 and name N)	5.71	0.09	0.09
	assign (segid 3A4 and resid 129 and name C)	(segid 3A4 and resid 132 and name C)	5.15	0.12	0.12
	assign (segid 3A4 and resid 129 and name C)	(segid 3A4 and resid 132 and name CA)	4.79	0.17	0.17
	assign (segid 3A4 and resid 129 and name C)	(segid 3A4 and resid 132 and name CB)	4.65	0.22	0.23
	assign (segid 3A4 and resid 129 and name C)	(segid 3A4 and resid 132 and name O)	3.98	0.18	0.17
80	assign (segid 3A4 and resid 129 and name C)	(segid 3A4 and resid 132 and name N)	6.36	0.11	0.12
	assign (segid 3A4 and resid 129 and name C)	(segid 3A4 and resid 133 and name C)	6.33	0.11	0.10
	assign (segid 3A4 and resid 129 and name C)	(segid 3A4 and resid 133 and name CA)	5.32	0.11	0.10
	assign (segid 3A4 and resid 129 and name C)	(segid 3A4 and resid 133 and name CB)	4.89	0.17	0.16

	assign (segid 3A4 and resid 129 and name C) (segid 3A4 and resid 133 and name CG1)	4.54	0.23	0.23
	assign (segid 3A4 and resid 129 and name C) (segid 3A4 and resid 133 and name CG2)	6.24	0.19	0.20
	assign (segid 3A4 and resid 129 and name C) (segid 3A4 and resid 133 and name N)	4.41	0.10	0.10
	assign (segid 3A4 and resid 129 and name C) (segid 3A4 and resid 133 and name O)	7.50	0.10	0.10
5	assign (segid 3A4 and resid 129 and name C) (segid 3A4 and resid 134 and name C)	7.38	0.15	0.15
	assign (segid 3A4 and resid 129 and name C) (segid 3A4 and resid 134 and name N)	6.11	0.12	0.13
	assign (segid 3A4 and resid 129 and name C) (segid 3A4 and resid 259 and name C)	7.60	0.18	0.18
	assign (segid 3A4 and resid 129 and name C) (segid 3A4 and resid 259 and name CB)	6.87	0.32	0.33
	assign (segid 3A4 and resid 129 and name C) (segid 3A4 and resid 260 and name CA)	7.41	0.22	0.21
	assign (segid 3A4 and resid 129 and name C) (segid 3A4 and resid 260 and name N)	7.28	0.29	0.29
10	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 129 and name C)	1.53	0.00	0.00
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 129 and name CB)	1.54	0.01	0.01
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 129 and name O)	2.38	0.02	0.02
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 130 and name C)	4.49	0.06	0.06
15	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 130 and name CB)	3.86	0.04	0.04
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 130 and name N)	4.85	0.07	0.07
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 130 and name O)	2.49	0.04	0.04
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 131 and name C)	5.45	0.09	0.09
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 131 and name CB)	5.59	0.14	0.14
20	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 131 and name CA)	5.50	0.08	0.08
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 131 and name CB)	5.97	0.11	0.12
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 131 and name N)	4.41	0.06	0.06
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 131 and name O)	6.73	0.14	0.14
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 132 and name C)	5.98	0.16	0.16
25	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 132 and name CA)	5.39	0.23	0.23
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 132 and name CB)	4.85	0.30	0.29
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 132 and name N)	4.72	0.21	0.21
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 132 and name O)	7.17	0.16	0.16
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 133 and name C)	7.58	0.14	0.13
30	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 133 and name CA)	6.44	0.13	0.12
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 133 and name CB)	6.08	0.18	0.18
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 133 and name CG1)	5.44	0.25	0.26
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 133 and name CG2)	7.45	0.21	0.21
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 133 and name N)	5.44	0.13	0.13
35	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 134 and name CA)	8.77	0.18	0.17
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 134 and name N)	7.47	0.16	0.16
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 135 and name CA)	10.06	0.18	0.17
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 135 and name CB)	9.66	0.22	0.21
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 136 and name CA)	10.90	0.19	0.19
40	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 136 and name CB)	10.22	0.23	0.24
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 137 and name CA)	12.41	0.40	0.40
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 138 and name CA)	14.36	0.24	0.24
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 138 and name CB)	14.10	0.21	0.20
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 139 and name CA)	15.02	0.65	0.64
45	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 140 and name CA)	14.09	0.54	0.54
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 140 and name CB)	13.76	0.40	0.41
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 141 and name CA)	13.65	1.47	1.48
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 141 and name CB)	14.62	1.98	1.98
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 147 and name CA)	14.01	1.61	1.61
50	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 147 and name CB)	14.53	2.22	2.21
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 148 and name CA)	15.30	0.66	0.66
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 149 and name CA)	13.95	1.16	1.17
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 149 and name CB)	14.04	1.66	1.66
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 150 and name CA)	12.25	1.05	1.04
55	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 151 and name CA)	13.74	1.53	1.54
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 152 and name CA)	14.74	1.12	1.13
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 152 and name CB)	15.08	1.74	1.75
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 153 and name CA)	13.31	1.23	1.23
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 153 and name CB)	12.77	1.31	1.31
60	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 154 and name CA)	13.13	1.90	1.89
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 155 and name CA)	15.62	1.45	1.45
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 155 and name CB)	16.23	1.28	1.27
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 156 and name CA)	15.95	1.64	1.64
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 156 and name CB)	15.60	2.09	2.10
65	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 157 and name CA)	14.97	1.60	1.60
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 157 and name CB)	13.97	1.75	1.76
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 219 and name CA)	17.31	0.97	0.97
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 219 and name CB)	16.80	0.98	0.98
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 220 and name CA)	17.45	0.98	0.99
70	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 220 and name CB)	16.39	1.00	1.00
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 221 and name CA)	18.86	0.80	0.80
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 250 and name CA)	16.87	1.75	1.75
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 251 and name CA)	14.13	1.81	1.82
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 251 and name CB)	14.36	1.91	1.91
75	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 252 and name CA)	11.97	1.82	1.82
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 252 and name CB)	12.61	1.87	1.86
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 253 and name CA)	13.09	1.45	1.45
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 254 and name CA)	13.30	1.45	1.45
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 255 and name CA)	10.18	1.57	1.57
80	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 256 and name CA)	7.99	1.59	1.59
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 257 and name CA)	10.07	1.30	1.30
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 258 and name CA)	11.06	1.06	1.07
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 258 and name CB)	11.83	1.18	1.17

	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 259 and name CA)	8.17	0.91	0.90
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 259 and name CB)	7.24	0.99	0.98
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 260 and name CA)	7.29	0.66	0.66
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 260 and name CB)	7.33	0.89	0.89
5	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 261 and name CA)	10.96	0.61	0.61
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 262 and name CA)	11.45	0.52	0.52
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 262 and name CB)	11.30	0.64	0.64
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 263 and name CA)	9.56	0.20	0.19
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 263 and name CB)	8.13	0.22	0.22
10	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 264 and name CA)	11.48	0.17	0.16
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 265 and name CA)	14.53	0.28	0.27
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 266 and name CA)	14.40	0.23	0.23
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 267 and name CA)	14.49	0.50	0.50
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 267 and name CB)	13.49	0.62	0.63
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 268 and name CA)	17.23	0.34	0.35
15	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 268 and name CB)	17.30	0.24	0.24
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 269 and name CA)	19.14	0.29	0.29
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 269 and name CB)	18.05	0.57	0.56
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 270 and name CA)	17.50	0.99	1.00
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 305 and name CB)	18.45	0.60	0.60
20	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 306 and name CA)	18.64	0.73	0.73
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 308 and name CB)	16.15	0.50	0.50
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 309 and name CA)	15.35	0.53	0.54
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 309 and name CB)	18.89	0.49	0.49
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 310 and name CA)	17.62	0.57	0.56
25	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 312 and name CA)	16.33	0.59	0.58
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 312 and name CB)	17.22	0.58	0.57
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 313 and name CA)	16.91	0.63	0.62
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 313 and name CB)	18.96	0.80	0.79
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 317 and name CA)	16.62	1.16	1.15
30	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 318 and name CA)	15.16	1.14	1.15
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 318 and name CB)	18.07	1.33	1.33
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 319 and name CA)	18.32	1.38	1.38
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 319 and name CB)	17.28	1.36	1.35
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 391 and name CA)	17.92	1.34	1.34
35	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 392 and name CA)	18.19	1.38	1.37
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 392 and name CB)	14.30	1.26	1.25
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 393 and name CA)	15.32	0.99	0.99
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 394 and name CA)	16.77	0.96	0.96
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 394 and name CB)	15.25	0.76	0.76
40	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 395 and name CA)	11.84	0.73	0.73
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 396 and name CA)	11.54	0.83	0.82
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 396 and name CB)	10.63	0.89	0.89
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 397 and name CA)	11.36	1.04	1.05
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 397 and name CB)	12.86	0.55	0.54
45	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 398 and name CA)	14.32	0.57	0.57
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 398 and name CB)	11.91	0.37	0.36
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 399 and name CA)	12.11	0.48	0.47
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 399 and name CB)	8.29	0.29	0.30
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 400 and name CA)	7.32	0.39	0.39
50	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 400 and name CB)	9.79	0.30	0.30
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 401 and name CA)	12.59	0.14	0.14
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 402 and name CA)	13.61	0.13	0.13
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 402 and name CB)	11.08	0.51	0.51
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 403 and name CA)	10.44	0.60	0.59
55	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 403 and name CB)	9.04	0.52	0.53
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 404 and name CA)	8.01	0.41	0.40
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 404 and name CB)	12.13	0.38	0.38
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 405 and name CA)	12.78	0.37	0.37
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 405 and name CB)	14.45	0.49	0.50
60	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 406 and name CA)	13.19	0.90	0.89
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 407 and name CA)	12.12	1.01	1.01
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 407 and name CB)	12.90	0.90	0.91
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 408 and name CA)	12.22	0.86	0.85
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 408 and name CB)	16.35	0.78	0.78
65	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 409 and name CA)	16.82	0.65	0.65
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 409 and name CB)	17.89	0.82	0.83
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 410 and name CA)	17.14	1.19	1.20
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 411 and name CA)	15.93	1.32	1.33
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 411 and name CB)	17.93	1.01	1.01
70	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 412 and name CA)	17.66	1.04	1.04
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 433 and name CA)	15.65	0.81	0.81
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 434 and name CA)	15.82	0.62	0.61
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 435 and name CA)	16.31	1.58	1.58
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 436 and name CA)	16.40	1.38	1.37
75	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 437 and name CA)	16.29	1.33	1.33
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 438 and name CA)	17.64	0.84	0.84
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 439 and name CA)	17.77	0.95	0.95
	assign (segid 3A4 and resid 129 and name CA) (segid 3A4 and resid 440 and name CA)	5.52	0.06	0.06
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 130 and name C)	4.54	0.08	0.09
80	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 130 and name CA)	5.30	0.17	0.17
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 130 and name CB)	3.19	0.08	0.08
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 130 and name N)	6.46	0.08	0.08
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 130 and name O)			

	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 131 and name C)	7.02	0.14	0.15
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 131 and name CA)	6.86	0.08	0.07
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 131 and name CB)	7.37	0.12	0.12
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 131 and name N)	5.64	0.08	0.08
5	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 132 and name C)	7.25	0.23	0.22
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 132 and name CA)	6.80	0.27	0.27
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 132 and name CB)	6.17	0.37	0.37
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 132 and name N)	6.19	0.22	0.23
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 133 and name CA)	7.36	0.19	0.19
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 133 and name CB)	6.73	0.23	0.23
10	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 133 and name CG1)	5.91	0.31	0.30
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 133 and name N)	6.56	0.20	0.20
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 134 and name CA)	9.84	0.18	0.18
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 135 and name CA)	11.40	0.19	0.19
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 135 and name CB)	11.09	0.23	0.23
15	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 136 and name CA)	12.03	0.26	0.26
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 136 and name CB)	11.25	0.29	0.29
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 137 and name CA)	13.34	0.48	0.49
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 138 and name CA)	15.49	0.31	0.31
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 138 and name CB)	15.25	0.22	0.22
20	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 139 and name CA)	16.30	0.65	0.65
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 140 and name CA)	15.50	0.58	0.58
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 140 and name CB)	15.16	0.45	0.46
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 141 and name CA)	15.11	1.48	1.48
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 141 and name CB)	16.09	1.97	1.98
25	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 147 and name CA)	15.18	1.32	1.32
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 147 and name CB)	15.65	1.95	1.96
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 148 and name CA)	16.47	0.77	0.77
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 149 and name CA)	15.14	1.54	1.55
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 149 and name CB)	15.27	2.02	2.01
30	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 150 and name CA)	13.33	0.66	0.65
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 151 and name CA)	14.71	1.17	1.17
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 152 and name CA)	15.70	1.49	1.50
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 152 and name CB)	16.10	2.18	2.18
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 153 and name CA)	14.16	1.59	1.60
35	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 153 and name CB)	13.65	1.66	1.67
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 154 and name CA)	13.85	1.42	1.41
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 155 and name CA)	16.26	1.28	1.27
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 155 and name CB)	16.92	1.26	1.25
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 156 and name CA)	16.54	2.04	2.03
40	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 157 and name CA)	15.40	1.61	1.60
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 157 and name CB)	14.42	1.59	1.59
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 219 and name CA)	18.31	1.01	1.01
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 219 and name CB)	17.88	1.02	1.02
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 220 and name CA)	18.33	1.11	1.10
45	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 220 and name CB)	17.22	1.14	1.14
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 251 and name CA)	14.63	2.21	2.22
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 251 and name CB)	14.95	2.25	2.25
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 252 and name CA)	12.63	2.26	2.26
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 252 and name CB)	13.38	2.27	2.27
50	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 253 and name CA)	13.47	2.01	2.01
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 254 and name CA)	13.38	1.99	1.99
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 255 and name CA)	10.30	2.04	2.04
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 256 and name CA)	8.13	2.20	2.19
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 257 and name CA)	9.87	1.95	1.95
55	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 258 and name CA)	10.55	1.62	1.62
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 258 and name CB)	11.35	1.70	1.70
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 259 and name CA)	7.51	1.33	1.33
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 259 and name CB)	6.70	1.40	1.39
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 260 and name CA)	6.67	1.10	1.11
60	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 260 and name CB)	6.91	1.39	1.39
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 261 and name CA)	10.18	1.00	0.99
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 262 and name CA)	10.47	0.76	0.76
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 262 and name CB)	10.34	0.86	0.87
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 263 and name CA)	8.49	0.25	0.26
65	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 263 and name CB)	7.10	0.30	0.31
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 263 and name CG)	6.53	0.42	0.41
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 264 and name CA)	10.50	0.23	0.23
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 265 and name CA)	13.46	0.39	0.39
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 266 and name CA)	13.22	0.30	0.31
70	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 267 and name CA)	13.35	0.66	0.67
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 267 and name CB)	12.40	0.80	0.80
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 268 and name CA)	16.13	0.37	0.37
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 268 and name CB)	16.22	0.19	0.20
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 269 and name CA)	17.94	0.36	0.37
75	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 270 and name CA)	17.87	0.72	0.71
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 270 and name CB)	16.84	0.80	0.79
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 271 and name CB)	18.35	0.89	0.89
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 305 and name CA)	17.30	1.13	1.13
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 305 and name CB)	16.46	1.27	1.27
80	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 306 and name CA)	17.44	0.73	0.73
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 308 and name CA)	17.91	0.74	0.75
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 308 and name CB)	17.45	0.87	0.87

5	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 309 and name CA)	15.04	0.53	0.52
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 309 and name CB)	14.30	0.56	0.56
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 310 and name CA)	17.84	0.50	0.49
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 312 and name CA)	16.45	0.58	0.59
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 312 and name CB)	15.15	0.59	0.59
10	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 313 and name CA)	16.18	0.67	0.67
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 313 and name CB)	15.92	0.72	0.72
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 316 and name CA)	17.77	0.79	0.80
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 317 and name CA)	18.04	1.06	1.06
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 318 and name CA)	15.83	1.53	1.54
15	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 318 and name CB)	14.39	1.52	1.52
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 319 and name CA)	17.79	1.68	1.68
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 319 and name CB)	17.50	1.78	1.77
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 384 and name CA)	18.21	1.36	1.37
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 384 and name CB)	17.86	1.33	1.33
20	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 391 and name CA)	18.03	1.69	1.69
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 391 and name CB)	16.92	1.66	1.66
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 392 and name CA)	17.85	1.58	1.58
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 393 and name CA)	14.21	1.45	1.45
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 394 and name CA)	14.92	1.13	1.13
25	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 394 and name CB)	16.33	1.09	1.10
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 395 and name CA)	14.93	0.75	0.75
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 396 and name CA)	11.72	0.71	0.70
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 396 and name CB)	11.57	0.83	0.83
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 397 and name CA)	10.18	0.95	0.96
30	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 397 and name CB)	10.87	1.19	1.18
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 398 and name CA)	12.17	0.47	0.48
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 398 and name CB)	13.64	0.50	0.49
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 399 and name CA)	11.41	0.31	0.32
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 399 and name CB)	11.77	0.42	0.41
35	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 400 and name CA)	7.79	0.35	0.36
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 400 and name CB)	6.92	0.34	0.33
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 401 and name CA)	8.87	0.28	0.28
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 402 and name CA)	11.69	0.50	0.50
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 402 and name CB)	12.78	0.46	0.46
40	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 403 and name CA)	10.37	1.03	1.03
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 403 and name CB)	9.87	1.11	1.10
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 404 and name CA)	8.15	1.11	1.11
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 404 and name CB)	7.07	0.93	0.92
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 405 and name CA)	11.06	0.73	0.73
45	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 405 and name CB)	11.66	0.58	0.59
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 406 and name CA)	13.50	1.00	1.01
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 407 and name CA)	12.40	1.52	1.52
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 407 and name CB)	11.43	1.66	1.66
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 408 and name CA)	12.00	1.49	1.49
50	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 408 and name CB)	11.24	1.40	1.41
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 409 and name CA)	15.35	1.31	1.31
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 409 and name CB)	15.77	1.14	1.14
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 410 and name CA)	17.04	1.41	1.41
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 411 and name CA)	16.42	1.78	1.78
55	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 411 and name CB)	15.27	1.93	1.93
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 433 and name CA)	16.99	1.38	1.38
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 434 and name CA)	14.94	1.04	1.03
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 435 and name CA)	15.09	0.43	0.42
	assign (segid 3A4 and resid 129 and name CB) (segid 3A4 and resid 436 and name CA)	15.81	1.29	1.29
60	assign (segid 3A4 and resid 129 and name CB			

5	assign	(segid 3A4 and resid 129 and name N)	(segid 3A4 and resid 260 and name CB)	6.99	0.75	0.74
	assign	(segid 3A4 and resid 129 and name O)	(segid 3A4 and resid 129 and name CB)	3.41	0.06	0.06
	assign	(segid 3A4 and resid 129 and name O)	(segid 3A4 and resid 130 and name C)	2.97	0.04	0.04
	assign	(segid 3A4 and resid 129 and name O)	(segid 3A4 and resid 130 and name CA)	2.73	0.02	0.03
	assign	(segid 3A4 and resid 129 and name O)	(segid 3A4 and resid 130 and name CB)	4.20	0.03	0.03
10	assign	(segid 3A4 and resid 129 and name O)	(segid 3A4 and resid 130 and name N)	2.24	0.02	0.02
	assign	(segid 3A4 and resid 129 and name O)	(segid 3A4 and resid 130 and name O)	3.54	0.10	0.10
	assign	(segid 3A4 and resid 129 and name O)	(segid 3A4 and resid 131 and name C)	4.11	0.14	0.15
	assign	(segid 3A4 and resid 129 and name O)	(segid 3A4 and resid 131 and name CA)	4.33	0.10	0.09
	assign	(segid 3A4 and resid 129 and name O)	(segid 3A4 and resid 131 and name CB)	5.33	0.16	0.16
15	assign	(segid 3A4 and resid 129 and name O)	(segid 3A4 and resid 131 and name N)	3.35	0.08	0.08
	assign	(segid 3A4 and resid 129 and name O)	(segid 3A4 and resid 131 and name O)	5.05	0.14	0.15
	assign	(segid 3A4 and resid 129 and name O)	(segid 3A4 and resid 132 and name C)	4.08	0.14	0.14
	assign	(segid 3A4 and resid 129 and name O)	(segid 3A4 and resid 132 and name CA)	3.95	0.20	0.20
	assign	(segid 3A4 and resid 129 and name O)	(segid 3A4 and resid 132 and name CB)	3.88	0.24	0.25
20	assign	(segid 3A4 and resid 129 and name O)	(segid 3A4 and resid 132 and name N)	3.38	0.21	0.22
	assign	(segid 3A4 and resid 129 and name O)	(segid 3A4 and resid 132 and name O)	5.26	0.13	0.14
	assign	(segid 3A4 and resid 129 and name O)	(segid 3A4 and resid 133 and name C)	5.24	0.12	0.12
	assign	(segid 3A4 and resid 129 and name O)	(segid 3A4 and resid 133 and name CA)	4.14	0.11	0.11
	assign	(segid 3A4 and resid 129 and name O)	(segid 3A4 and resid 133 and name CB)	3.81	0.15	0.15
25	assign	(segid 3A4 and resid 129 and name O)	(segid 3A4 and resid 133 and name CG1)	3.48	0.19	0.19
	assign	(segid 3A4 and resid 129 and name O)	(segid 3A4 and resid 133 and name CG2)	5.23	0.17	0.17
	assign	(segid 3A4 and resid 129 and name O)	(segid 3A4 and resid 133 and name N)	3.26	0.12	0.12
	assign	(segid 3A4 and resid 129 and name O)	(segid 3A4 and resid 133 and name O)	6.38	0.12	0.12
	assign	(segid 3A4 and resid 129 and name O)	(segid 3A4 and resid 134 and name C)	7.37	0.13	0.14
30	assign	(segid 3A4 and resid 129 and name O)	(segid 3A4 and resid 134 and name CA)	6.53	0.15	0.16
	assign	(segid 3A4 and resid 129 and name O)	(segid 3A4 and resid 134 and name N)	5.18	0.14	0.15
	assign	(segid 3A4 and resid 129 and name O)	(segid 3A4 and resid 135 and name N)	7.01	0.13	0.14
	assign	(segid 3A4 and resid 12 and name C)	(segid 3A4 and resid 12 and name CB)	2.51	0.01	0.02
	assign	(segid 3A4 and resid 12 and name C)	(segid 3A4 and resid 12 and name O)	1.23	0.01	0.01
35	assign	(segid 3A4 and resid 12 and name C)	(segid 3A4 and resid 13 and name C)	3.08	0.08	0.09
	assign	(segid 3A4 and resid 12 and name C)	(segid 3A4 and resid 13 and name CA)	2.45	0.01	0.01
	assign	(segid 3A4 and resid 12 and name C)	(segid 3A4 and resid 13 and name CB)	3.70	0.03	0.03
	assign	(segid 3A4 and resid 12 and name C)	(segid 3A4 and resid 13 and name N)	1.33	0.00	0.01
	assign	(segid 3A4 and resid 12 and name C)	(segid 3A4 and resid 13 and name O)	3.93	0.16	0.15
40	assign	(segid 3A4 and resid 12 and name CA)	(segid 3A4 and resid 12 and name C)	1.53	0.01	0.01
	assign	(segid 3A4 and resid 12 and name CA)	(segid 3A4 and resid 12 and name CB)	1.53	0.00	0.01
	assign	(segid 3A4 and resid 12 and name CA)	(segid 3A4 and resid 12 and name O)	2.40	0.01	0.02
	assign	(segid 3A4 and resid 12 and name CA)	(segid 3A4 and resid 13 and name C)	4.48	0.06	0.06
	assign	(segid 3A4 and resid 12 and name CA)	(segid 3A4 and resid 13 and name CA)	3.82	0.01	0.02
45	assign	(segid 3A4 and resid 12 and name CA)	(segid 3A4 and resid 13 and name CB)	4.84	0.03	0.03
	assign	(segid 3A4 and resid 12 and name CA)	(segid 3A4 and resid 13 and name N)	2.44	0.01	0.01
	assign	(segid 3A4 and resid 12 and name CA)	(segid 3A4 and resid 13 and name O)	5.39	0.15	0.15
	assign	(segid 3A4 and resid 12 and name CA)	(segid 3A4 and resid 19 and name CA)	9.66	2.13	2.13
	assign	(segid 3A4 and resid 12 and name CA)	(segid 3A4 and resid 19 and name CB)	10.68	2.38	2.37
50	assign	(segid 3A4 and resid 12 and name CA)	(segid 3A4 and resid 20 and name CA)	11.75	1.42	1.42
	assign	(segid 3A4 and resid 12 and name CA)	(segid 3A4 and resid 20 and name CB)	13.15	1.55	1.55
	assign	(segid 3A4 and resid 12 and name CA)	(segid 3A4 and resid 21 and name CA)	11.53	0.71	0.71
	assign	(segid 3A4 and resid 12 and name CA)	(segid 3A4 and resid 21 and name CB)	10.30	0.55	0.55
	assign	(segid 3A4 and resid 12 and name CA)	(segid 3A4 and resid 22 and name CA)	13.82	0.52	0.52
55	assign	(segid 3A4 and resid 12 and name CA)	(segid 3A4 and resid 23 and name CA)	13.51	0.47	0.47

assign (segid 3A4 and resid 12 and name CA) (segid 3A4 and resid 351 and name CA) 14.37 1.20 1.20
 assign (segid 3A4 and resid 12 and name CA) (segid 3A4 and resid 352 and name CA) 11.85 1.26 1.27
 assign (segid 3A4 and resid 12 and name CA) (segid 3A4 and resid 352 and name CB) 10.97 1.14 1.13
 assign (segid 3A4 and resid 12 and name CA) (segid 3A4 and resid 353 and name CA) 11.60 1.90 1.91
 assign (segid 3A4 and resid 12 and name CA) (segid 3A4 and resid 353 and name CB) 12.23 2.09 2.10
 assign (segid 3A4 and resid 12 and name CA) (segid 3A4 and resid 354 and name CA) 12.88 1.95 1.96
 assign (segid 3A4 and resid 12 and name CA) (segid 3A4 and resid 354 and name CB) 12.29 1.94 1.95
 assign (segid 3A4 and resid 12 and name CA) (segid 3A4 and resid 355 and name CA) 15.08 2.49 2.49
 assign (segid 3A4 and resid 12 and name CA) (segid 3A4 and resid 355 and name CB) 14.89 2.71 2.70
 assign (segid 3A4 and resid 12 and name CA) (segid 3A4 and resid 356 and name CA) 16.50 2.12 2.11
 assign (segid 3A4 and resid 12 and name CA) (segid 3A4 and resid 357 and name CB) 16.49 1.61 1.60
 assign (segid 3A4 and resid 12 and name CA) (segid 3A4 and resid 359 and name CA) 16.27 1.43 1.44
 assign (segid 3A4 and resid 12 and name CA) (segid 3A4 and resid 359 and name CB) 17.57 1.36 1.35
 assign (segid 3A4 and resid 12 and name CA) (segid 3A4 and resid 35 and name CA) 11.35 2.10 2.11
 assign (segid 3A4 and resid 12 and name CA) (segid 3A4 and resid 360 and name CA) 14.46 1.27 1.27
 assign (segid 3A4 and resid 12 and name CA) (segid 3A4 and resid 360 and name CB) 13.29 1.31 1.30
 assign (segid 3A4 and resid 12 and name CA) (segid 3A4 and resid 361 and name CA) 14.21 1.09 1.09
 assign (segid 3A4 and resid 12 and name CA) (segid 3A4 and resid 361 and name CB) 13.41 1.11 1.11
 assign (segid 3A4 and resid 12 and name CA) (segid 3A4 and resid 36 and name CA) 14.46 2.06 2.05
 assign (segid 3A4 and resid 12 and name CA) (segid 3A4 and resid 37 and name CA) 16.57 2.19 2.19
 assign (segid 3A4 and resid 12 and name CA) (segid 3A4 and resid 37 and name CB) 16.50 2.28 2.27
 assign (segid 3A4 and resid 12 and name CA) (segid 3A4 and resid 38 and name CA) 15.81 2.04 2.03
 assign (segid 3A4 and resid 12 and name CA) (segid 3A4 and resid 38 and name CB) 14.67 2.02 2.02
 assign (segid 3A4 and resid 12 and name CA) (segid 3A4 and resid 39 and name CA) 16.23 1.74 1.75
 assign (segid 3A4 and resid 12 and name CA) (segid 3A4 and resid 39 and name CB) 15.48 1.64 1.64
 assign (segid 3A4 and resid 12 and name CA) (segid 3A4 and resid 430 and name CA) 17.96 1.03 1.03
 assign (segid 3A4 and resid 12 and name CA) (segid 3A4 and resid 13 and name C) 5.49 0.07 0.08
 assign (segid 3A4 and resid 12 and name CB) (segid 3A4 and resid 13 and name CA) 4.50 0.08 0.08
 assign (segid 3A4 and resid 12 and name CB) (segid 3A4 and resid 13 and name CB) 5.32 0.12 0.13
 assign (segid 3A4 and resid 12 and name CB) (segid 3A4 and resid 13 and name N) 3.18 0.09 0.08
 assign (segid 3A4 and resid 12 and name CB) (segid 3A4 and resid 13 and name O) 6.37 0.17 0.17
 assign (segid 3A4 and resid 12 and name CB) (segid 3A4 and resid 19 and name CA) 10.84 2.14 2.15
 assign (segid 3A4 and resid 12 and name CB) (segid 3A4 and resid 19 and name CB) 11.90 2.43 2.43
 assign (segid 3A4 and resid 12 and name CB) (segid 3A4 and resid 20 and name CA) 12.68 1.39 1.39
 assign (segid 3A4 and resid 12 and name CB) (segid 3A4 and resid 20 and name CB) 14.11 1.53 1.53
 assign (segid 3A4 and resid 12 and name CB) (segid 3A4 and resid 21 and name CA) 12.17 0.56 0.56
 assign (segid 3A4 and resid 12 and name CB) (segid 3A4 and resid 21 and name CB) 10.89 0.39 0.40
 assign (segid 3A4 and resid 12 and name CB) (segid 3A4 and resid 22 and name CA) 14.16 0.47 0.48
 assign (segid 3A4 and resid 12 and name CB) (segid 3A4 and resid 23 and name CA) 13.51 0.69 0.70
 assign (segid 3A4 and resid 12 and name CB) (segid 3A4 and resid 23 and name CB) 12.67 0.80 0.79
 assign (segid 3A4 and resid 12 and name CB) (segid 3A4 and resid 24 and name CA) 16.46 0.91 0.91
 assign (segid 3A4 and resid 12 and name CB) (segid 3A4 and resid 24 and name CB) 17.12 1.00 1.01
 assign (segid 3A4 and resid 12 and name CB) (segid 3A4 and resid 29 and name CA) 18.91 0.61 0.61
 assign (segid 3A4 and resid 12 and name CB) (segid 3A4 and resid 30 and name CA) 17.20 0.43 0.43
 assign (segid 3A4 and resid 12 and name CB) (segid 3A4 and resid 317 and name CA) 17.48 1.10 1.11
 assign (segid 3A4 and resid 12 and name CB) (segid 3A4 and resid 31 and name CA) 15.39 0.53 0.53
 assign (segid 3A4 and resid 12 and name CB) (segid 3A4 and resid 31 and name CB) 16.27 0.73 0.73
 assign (segid 3A4 and resid 12 and name CB) (segid 3A4 and resid 32 and name CA) 12.68 0.64 0.64
 assign (segid 3A4 and resid 12 and name CB) (segid 3A4 and resid 32 and name CB) 11.48 0.40 0.41
 assign (segid 3A4 and resid 12 and name CB) (segid 3A4 and resid 33 and name CA) 13.05 1.53 1.53
 assign (segid 3A4 and resid 12 and name CB) (segid 3A4 and resid 33 and name CB) 14.38 1.68 1.69
 assign (segid 3A4 and resid 12 and name CB) (segid 3A4 and resid 343 and name CA) 18.20 0.83 0.83
 assign (segid 3A4 and resid 12 and name CB) (segid 3A4 and resid 343 and name CB) 18.65 0.99 1.00
 assign (segid 3A4 and resid 12 and name CB) (segid 3A4 and resid 344 and name CA) 16.00 0.77 0.77
 assign (segid 3A4 and resid 12 and name CB) (segid 3A4 and resid 344 and name CB) 15.20 0.65 0.65
 assign (segid 3A4 and resid 12 and name CB) (segid 3A4 and resid 345 and name CA) 15.47 1.29 1.28
 assign (segid 3A4 and resid 12 and name CB) (segid 3A4 and resid 345 and name CB) 16.69 1.47 1.48
 assign (segid 3A4 and resid 12 and name CB) (segid 3A4 and resid 346 and name CA) 13.03 1.06 1.07
 assign (segid 3A4 and resid 12 and name CB) (segid 3A4 and resid 346 and name CB) 11.68 0.91 0.91
 assign (segid 3A4 and resid 12 and name CB) (segid 3A4 and resid 347 and name CA) 15.16 1.39 1.40
 assign (segid 3A4 and resid 12 and name CB) (segid 3A4 and resid 347 and name CB) 16.44 1.36 1.35
 assign (segid 3A4 and resid 12 and name CB) (segid 3A4 and resid 348 and name CA) 13.24 1.06 1.05
 assign (segid 3A4 and resid 12 and name CB) (segid 3A4 and resid 349 and name CA) 10.78 1.41 1.42
 assign (segid 3A4 and resid 12 and name CB) (segid 3A4 and resid 349 and name CB) 10.06 1.41 1.40
 assign (segid 3A4 and resid 12 and name CB) (segid 3A4 and resid 34 and name CA) 10.55 1.91 1.91
 assign (segid 3A4 and resid 12 and name CB) (segid 3A4 and resid 34 and name CB) 9.26 1.83 1.83
 assign (segid 3A4 and resid 12 and name CB) (segid 3A4 and resid 350 and name CA) 13.59 2.15 2.14
 assign (segid 3A4 and resid 12 and name CB) (segid 3A4 and resid 350 and name CB) 14.74 2.14 2.15
 assign (segid 3A4 and resid 12 and name CB) (segid 3A4 and resid 351 and name CA) 15.11 1.84 1.83
 assign (segid 3A4 and resid 12 and name CB) (segid 3A4 and resid 352 and name CA) 12.57 1.84 1.85
 assign (segid 3A4 and resid 12 and name CB) (segid 3A4 and resid 352 and name CB) 11.62 1.62 1.61
 assign (segid 3A4 and resid 12 and name CB) (segid 3A4 and resid 353 and name CA) 12.53 2.58 2.58
 assign (segid 3A4 and resid 12 and name CB) (segid 3A4 and resid 353 and name CB) 13.21 2.75 2.74
 assign (segid 3A4 and resid 12 and name CB) (segid 3A4 and resid 354 and name CA) 13.81 2.55 2.56
 assign (segid 3A4 and resid 12 and name CB) (segid 3A4 and resid 354 and name CB) 13.22 2.51 2.51
 assign (segid 3A4 and resid 12 and name CB) (segid 3A4 and resid 359 and name CA) 16.89 1.80 1.81
 assign (segid 3A4 and resid 12 and name CB) (segid 3A4 and resid 35 and name CA) 12.44 2.59 2.58
 assign (segid 3A4 and resid 12 and name CB) (segid 3A4 and resid 360 and name CA) 15.09 1.72 1.72
 assign (segid 3A4 and resid 12 and name CB) (segid 3A4 and resid 360 and name CB) 13.97 1.82 1.82
 assign (segid 3A4 and resid 12 and name CB) (segid 3A4 and resid 361 and name CA) 14.59 1.26 1.27
 assign (segid 3A4 and resid 12 and name CB) (segid 3A4 and resid 361 and name CB) 13.74 1.22 1.23
 assign (segid 3A4 and resid 12 and name CB) (segid 3A4 and resid 36 and name CA) 15.49 2.62 2.61
 assign (segid 3A4 and resid 12 and name CB) (segid 3A4 and resid 38 and name CB) 15.74 2.29 2.30

	assign (segid 3A4 and resid 12 and name CB)	(segid 3A4 and resid 39 and name CB)	16.39	2.09	2.08
	assign (segid 3A4 and resid 12 and name CB)	(segid 3A4 and resid 430 and name CA)	17.69	0.99	0.99
	assign (segid 3A4 and resid 12 and name N)	(segid 3A4 and resid 12 and name C)	2.42	0.05	0.05
	assign (segid 3A4 and resid 12 and name N)	(segid 3A4 and resid 12 and name CA)	1.46	0.01	0.00
5	assign (segid 3A4 and resid 12 and name N)	(segid 3A4 and resid 12 and name CB)	2.48	0.05	0.04
	assign (segid 3A4 and resid 12 and name N)	(segid 3A4 and resid 12 and name O)	3.46	0.07	0.08
	assign (segid 3A4 and resid 12 and name N)	(segid 3A4 and resid 13 and name C)	4.68	0.06	0.07
	assign (segid 3A4 and resid 12 and name N)	(segid 3A4 and resid 13 and name CA)	4.15	0.06	0.05
	assign (segid 3A4 and resid 12 and name N)	(segid 3A4 and resid 13 and name CB)	4.86	0.08	0.08
	assign (segid 3A4 and resid 12 and name N)	(segid 3A4 and resid 13 and name N)	2.75	0.06	0.05
10	assign (segid 3A4 and resid 12 and name N)	(segid 3A4 and resid 13 and name O)	5.77	0.11	0.10
	assign (segid 3A4 and resid 12 and name O)	(segid 3A4 and resid 12 and name CB)	3.29	0.08	0.09
	assign (segid 3A4 and resid 12 and name O)	(segid 3A4 and resid 13 and name C)	3.07	0.15	0.15
	assign (segid 3A4 and resid 12 and name O)	(segid 3A4 and resid 13 and name CA)	2.79	0.02	0.03
	assign (segid 3A4 and resid 12 and name O)	(segid 3A4 and resid 13 and name CB)	4.25	0.04	0.05
15	assign (segid 3A4 and resid 12 and name O)	(segid 3A4 and resid 13 and name N)	2.25	0.00	0.00
	assign (segid 3A4 and resid 12 and name O)	(segid 3A4 and resid 13 and name O)	3.57	0.26	0.26
	assign (segid 3A4 and resid 12 and name O)	(segid 3A4 and resid 130 and name CB)	2.51	0.03	0.03
	assign (segid 3A4 and resid 130 and name C)	(segid 3A4 and resid 130 and name O)	1.25	0.02	0.01
	assign (segid 3A4 and resid 130 and name C)	(segid 3A4 and resid 131 and name C)	3.05	0.04	0.04
20	assign (segid 3A4 and resid 130 and name C)	(segid 3A4 and resid 131 and name CA)	2.41	0.03	0.03
	assign (segid 3A4 and resid 130 and name C)	(segid 3A4 and resid 131 and name CB)	3.70	0.04	0.03
	assign (segid 3A4 and resid 130 and name C)	(segid 3A4 and resid 131 and name N)	1.32	0.02	0.02
	assign (segid 3A4 and resid 130 and name C)	(segid 3A4 and resid 131 and name O)	3.88	0.06	0.05
	assign (segid 3A4 and resid 130 and name C)	(segid 3A4 and resid 132 and name C)	4.68	0.05	0.05
25	assign (segid 3A4 and resid 130 and name C)	(segid 3A4 and resid 132 and name CA)	4.59	0.05	0.06
	assign (segid 3A4 and resid 130 and name C)	(segid 3A4 and resid 132 and name CB)	5.39	0.08	0.08
	assign (segid 3A4 and resid 130 and name C)	(segid 3A4 and resid 132 and name N)	3.41	0.07	0.07
	assign (segid 3A4 and resid 130 and name C)	(segid 3A4 and resid 132 and name O)	5.75	0.06	0.07
	assign (segid 3A4 and resid 130 and name C)	(segid 3A4 and resid 133 and name C)	4.93	0.05	0.05
30	assign (segid 3A4 and resid 130 and name C)	(segid 3A4 and resid 133 and name CA)	4.67	0.09	0.08
	assign (segid 3A4 and resid 130 and name C)	(segid 3A4 and resid 133 and name CB)	4.51	0.16	0.16
	assign (segid 3A4 and resid 130 and name C)	(segid 3A4 and resid 133 and name CG1)	5.14	0.19	0.20
	assign (segid 3A4 and resid 130 and name C)	(segid 3A4 and resid 133 and name CG2)	5.64	0.17	0.18
	assign (segid 3A4 and resid 130 and name C)	(segid 3A4 and resid 133 and name N)	3.95	0.05	0.05
35	assign (segid 3A4 and resid 130 and name C)	(segid 3A4 and resid 133 and name O)	6.12	0.05	0.06
	assign (segid 3A4 and resid 130 and name C)	(segid 3A4 and resid 134 and name C)	6.06	0.07	0.08
	assign (segid 3A4 and resid 130 and name C)	(segid 3A4 and resid 134 and name CA)	5.03	0.13	0.12
	assign (segid 3A4 and resid 130 and name C)	(segid 3A4 and resid 134 and name N)	4.14	0.07	0.07
	assign (segid 3A4 and resid 130 and name C)	(segid 3A4 and resid 134 and name O)	7.25	0.10	0.09
40	assign (segid 3A4 and resid 130 and name C)	(segid 3A4 and resid 135 and name CA)	7.18	0.06	0.06
	assign (segid 3A4 and resid 130 and name C)	(segid 3A4 and resid 135 and name CB)	7.20	0.10	0.11
	assign (segid 3A4 and resid 130 and name C)	(segid 3A4 and resid 135 and name N)	5.91	0.05	0.05
	assign (segid 3A4 and resid 130 and name C)	(segid 3A4 and resid 136 and name N)	7.84	0.04	0.05
	assign (segid 3A4 and resid 130 and name C)	(segid 3A4 and resid 256 and name C)	6.71	0.69	0.69
45	assign (segid 3A4 and resid 130 and name C)	(segid 3A4 and resid 256 and name CA)	5.91	0.67	0.67
	assign (segid 3A4 and resid 130 and name C)	(segid 3A4 and resid 256 and name N)	6.65	0.62	0.63
	assign (segid 3A4 and resid 130 and name C)	(segid 3A4 and resid 256 and name O)	6.57	0.75	0.74
	assign (segid 3A4 and resid 130 and name CA)	(segid 3A4 and resid 130 and name C)	1.52	0.01	0.01
	assign (segid 3A4 and resid 130 and name CA)	(segid 3A4 and resid 130 and name CB)	1.53	0.01	0.00
50	assign (segid 3A4 and resid 130 and name CA)	(segid 3A4 and resid 130 and name O)	2.41	0.02	0.01
	assign (segid 3A4 and resid 130 and name CA)	(segid 3A4 and resid 131 and name C)	4.43	0.06	0.05
	assign (segid 3A4 and resid 130 and name CA)	(segid 3A4 and resid 131 and name CA)	3.79	0.05	0.04
	assign (segid 3A4 and resid 130 and name CA)	(segid 3A4 and resid 131 and name CB)	4.86	0.05	0.05
	assign (segid 3A4 and resid 130 and name CA)	(segid 3A4 and resid 131 and name N)	2.43	0.03	0.03
55	assign (segid 3A4 and resid 130 and name CA)	(segid 3A4 and resid 131 and name O)	5.33	0.06	0.06
	assign (segid 3A4 and resid 130 and name CA)	(segid 3A4 and resid 132 and name C)	5.64	0.05	0.06
	assign (segid 3A4 and resid 130 and name CA)	(segid 3A4 and resid 132 and name CA)	5.59	0.08	0.08
	assign (segid 3A4 and resid 130 and name CA)	(segid 3A4 and resid 132 and name CB)	6.07	0.13	0.13
	assign (segid 3A4 and resid 130 and name CA)	(segid 3A4 and resid 132 and name N)	4.49	0.10	0.10
60	assign (segid 3A4 and resid 130 and name CA)	(segid 3A4 and resid 132 and name O)	6.77	0.06	0.06
	assign (segid 3A4 and resid 130 and name CA)	(segid 3A4 and resid 133 and name C)	5.80	0.06	0.05
	assign (segid 3A4 and resid 130 and name CA)	(segid 3A4 and resid 133 and name CA)	5.29	0.11	0.12
	assign (segid 3A4 and resid 130 and name CA)	(segid 3A4 and resid 133 and name CB)	4.71	0.21	0.22
	assign (segid 3A4 and resid 130 and name CA)	(segid 3A4 and resid 133 and name CG1)	5.05	0.27	0.27
65	assign (segid 3A4 and resid 130 and name CA)	(segid 3A4 and resid 133 and name CG2)	5.77	0.25	0.25
	assign (segid 3A4 and resid 130 and name CA)	(segid 3A4 and resid 133 and name N)	4.72	0.07	0.07
	assign (segid 3A4 and resid 130 and name CA)	(segid 3A4 and resid 133 and name O)	6.98	0.04	0.04
	assign (segid 3A4 and resid 130 and name CA)	(segid 3A4 and resid 134 and name C)	7.34	0.06	0.06
	assign (segid 3A4 and resid 130 and name CA)	(segid 3A4 and resid 134 and name CA)	6.17	0.09	0.08
70	assign (segid 3A4 and resid 130 and name CA)	(segid 3A4 and resid 134 and name N)	5.19	0.05	0.06
	assign (segid 3A4 and resid 130 and name CA)	(segid 3A4 and resid 135 and name CA)	8.58	0.06	0.06
	assign (segid 3A4 and resid 130 and name CA)	(segid 3A4 and resid 135 and name CB)	8.63	0.10	0.10
	assign (segid 3A4 and resid 130 and name CA)	(segid 3A4 and resid 135 and name N)	7.28	0.06	0.05
	assign (segid 3A4 and resid 130 and name CA)	(segid 3A4 and resid 136 and name CA)	10.04	0.07	0.08
75	assign (segid 3A4 and resid 130 and name CA)	(segid 3A4 and resid 136 and name CB)	9.74	0.23	0.23
	assign (segid 3A4 and resid 130 and name CA)	(segid 3A4 and resid 137 and name CA)	10.54	0.20	0.20
	assign (segid 3A4 and resid 130 and name CA)	(segid 3A4 and resid 138 and name CA)	12.10	0.21	0.22
	assign (segid 3A4 and resid 130 and name CA)	(segid 3A4 and resid 138 and name CB)	11.66	0.26	0.27
	assign (segid 3A4 and resid 130 and name CA)	(segid 3A4 and resid 139 and name CA)	13.48	0.74	0.75
80	assign (segid 3A4 and resid 130 and name CA)	(segid 3A4 and resid 140 and name CA)	12.56	0.98	0.98
	assign (segid 3A4 and resid 130 and name CA)	(segid 3A4 and resid 140 and name CB)	12.02	0.73	0.72
	assign (segid 3A4 and resid 130 and name CA)	(segid 3A4 and resid 141 and name CA)	12.82	2.18	2.18

	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 141 and name CB)	13.96	2.52	2.52
	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 147 and name CA)	13.32	0.69	0.69
	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 147 and name CB)	14.06	1.01	1.01
	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 148 and name CA)	14.53	1.75	1.74
	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 149 and name CA)	12.70	2.39	2.39
5	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 149 and name CB)	12.64	2.75	2.75
	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 150 and name CA)	11.21	0.50	0.49
	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 151 and name CA)	12.83	0.86	0.85
	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 152 and name CA)	13.34	2.06	2.06
	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 152 and name CB)	13.62	2.83	2.83
10	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 153 and name CA)	11.56	1.63	1.64
	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 153 and name CB)	10.99	1.60	1.59
	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 154 and name CA)	11.63	1.30	1.31
	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 155 and name CA)	14.15	1.22	1.22
	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 155 and name CB)	14.84	1.32	1.33
15	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 156 and name CA)	14.11	1.84	1.84
	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 156 and name CB)	13.70	2.34	2.34
	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 157 and name CA)	12.95	1.58	1.58
	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 157 and name CB)	11.88	1.75	1.75
	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 158 and name CA)	14.58	1.99	2.00
20	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 158 and name CB)	14.63	2.11	2.11
	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 159 and name CA)	17.12	1.40	1.41
	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 159 and name CB)	17.39	1.45	1.45
	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 160 and name CA)	17.19	1.55	1.55
	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 160 and name CB)	16.48	1.68	1.69
25	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 194 and name CA)	16.57	2.13	2.12
	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 194 and name CB)	15.83	1.95	1.94
	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 197 and name CB)	16.62	2.26	2.27
	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 198 and name CA)	17.14	2.03	2.03
	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 198 and name CB)	16.74	1.92	1.92
30	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 201 and name CB)	17.33	1.80	1.80
	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 219 and name CA)	15.77	0.57	0.56
	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 219 and name CB)	15.24	0.73	0.73
	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 220 and name CA)	15.40	0.40	0.40
	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 220 and name CB)	14.22	0.38	0.38
35	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 221 and name CA)	16.97	0.60	0.61
	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 221 and name CB)	16.59	0.68	0.67
	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 247 and name CA)	17.07	1.29	1.30
	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 247 and name CB)	17.70	1.21	1.20
40	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 248 and name CA)	14.48	1.57	1.58
	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 248 and name CB)	14.97	1.69	1.68
	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 249 and name CA)	14.10	1.63	1.63
	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 250 and name CA)	13.93	1.01	1.01
	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 250 and name CB)	15.09	0.89	0.89
	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 251 and name CA)	11.33	0.88	0.89
45	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 251 and name CB)	11.62	1.03	1.02
	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 252 and name CA)	9.10	1.37	1.37
	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 252 and name CB)	9.70	1.70	1.69
	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 253 and name CA)	10.33	0.84	0.84
	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 254 and name CA)	10.71	0.45	0.45
50	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 255 and name C)	6.70	0.53	0.54
	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 255 and name CA)	7.82	0.56	0.56
	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 255 and name O)	6.13	0.82	0.83
	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 256 and name C)	6.37	0.56	0.57
	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 256 and name CA)	5.78	0.69	0.69
55	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 256 and name N)	6.61	0.50	0.50
	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 256 and name O)	6.08	0.67	0.68
	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 257 and name CA)	8.41	0.46	0.46
	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 258 and name CA)	9.63	0.74	0.74
	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 258 and name CB)	10.21	0.72	0.71
60	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 259 and name CA)	7.30	1.21	1.22
	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 259 and name CB)	6.21	1.30	1.30
	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 260 and name CA)	7.17	0.90	0.91
	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 260 and name CB)	7.03	0.52	0.53
	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 261 and name CA)	10.74	0.80	0.80
65	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 262 and name CA)	11.49	1.23	1.23
	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 262 and name CB)	11.16	1.30	1.31
	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 263 and name CA)	10.53	1.39	1.40
	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 263 and name CB)	9.28	1.40	1.41
	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 264 and name CA)	12.53	0.98	0.98
70	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 265 and name CA)	15.22	1.10	1.10
	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 266 and name CA)	15.51	1.42	1.41
	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 267 and name CA)	16.17	1.37	1.37
	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 267 and name CB)	15.30	1.35	1.35
	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 309 and name CB)	15.91	1.77	1.78
75	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 312 and name CB)	16.85	1.79	1.79
	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 313 and name CB)	16.55	1.69	1.70
	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 318 and name CA)	15.69	1.05	1.04
	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 318 and name CB)	14.29	1.10	1.10
	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 319 and name CA)	16.92	0.99	1.00
80	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 319 and name CB)	16.44	0.93	0.94
	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 384 and name CA)	17.36	1.02	1.03
	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 384 and name CB)	17.05	1.09	1.10

	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 391 and name CA)	16.34	0.63	0.62
	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 391 and name CB)	15.43	0.71	0.71
	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 392 and name CA)	15.84	0.63	0.63
	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 392 and name CB)	15.94	0.59	0.60
5	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 393 and name CA)	12.42	0.74	0.75
	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 394 and name CA)	13.96	1.11	1.12
	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 394 and name CB)	15.42	1.13	1.13
	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 395 and name CA)	14.29	1.22	1.22
	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 396 and name CA)	10.83	1.24	1.25
	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 396 and name CB)	10.24	1.11	1.11
10	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 397 and name CA)	9.74	1.29	1.30
	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 397 and name CB)	10.30	1.17	1.17
	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 398 and name CA)	12.66	1.49	1.49
	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 398 and name CB)	14.07	1.46	1.45
	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 399 and name CA)	12.12	1.57	1.58
15	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 399 and name CB)	12.17	1.51	1.50
	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 400 and name CA)	8.79	1.61	1.62
	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 400 and name CB)	7.48	1.64	1.63
	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 401 and name CA)	10.59	1.60	1.60
	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 402 and name CA)	13.75	1.62	1.62
20	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 402 and name CB)	14.60	1.66	1.66
	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 403 and name CA)	12.74	1.57	1.57
	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 403 and name CB)	11.99	1.59	1.58
	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 404 and name CA)	11.16	1.35	1.35
	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 404 and name CB)	10.00	1.28	1.28
25	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 405 and name CA)	14.15	1.19	1.20
	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 405 and name CB)	14.57	1.23	1.23
	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 406 and name CA)	16.61	1.34	1.35
	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 407 and name CA)	15.79	1.32	1.32
	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 407 and name CB)	14.75	1.35	1.35
30	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 408 and name CA)	15.65	1.21	1.21
	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 408 and name CB)	14.86	1.23	1.23
	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 433 and name CA)	16.85	1.00	0.99
	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 434 and name CA)	15.26	0.91	0.90
	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 435 and name CA)	16.13	1.38	1.38
35	assign (segid 3A4 and resid 130 and name CA) (segid 3A4 and resid 131 and name C)	5.47	0.07	0.08
	assign (segid 3A4 and resid 130 and name CB) (segid 3A4 and resid 131 and name CA)	4.49	0.09	0.09
	assign (segid 3A4 and resid 130 and name CB) (segid 3A4 and resid 131 and name CB)	5.35	0.10	0.09
	assign (segid 3A4 and resid 130 and name CB) (segid 3A4 and resid 131 and name N)	3.18	0.08	0.09
	assign (segid 3A4 and resid 130 and name CB) (segid 3A4 and resid 131 and name O)	6.32	0.05	0.06
40	assign (segid 3A4 and resid 130 and name CB) (segid 3A4 and resid 132 and name C)	7.05	0.05	0.06
	assign (segid 3A4 and resid 130 and name CB) (segid 3A4 and resid 132 and name CA)	6.95	0.08	0.09
	assign (segid 3A4 and resid 130 and name CB) (segid 3A4 and resid 132 and name CB)	7.50	0.13	0.12
	assign (segid 3A4 and resid 130 and name CB) (segid 3A4 and resid 132 and name N)	5.74	0.11	0.10
	assign (segid 3A4 and resid 130 and name CB) (segid 3A4 and resid 133 and name C)	6.97	0.04	0.04
45	assign (segid 3A4 and resid 130 and name CB) (segid 3A4 and resid 133 and name CA)	6.64	0.10	0.11
	assign (segid 3A4 and resid 130 and name CB) (segid 3A4 and resid 133 and name CB)	5.99	0.21	0.21
	assign (segid 3A4 and resid 130 and name CB) (segid 3A4 and resid 133 and name CG1)	6.41	0.28	0.27
	assign (segid 3A4 and resid 130 and name CB) (segid 3A4 and resid 133 and name CG2)	6.85	0.26	0.27
	assign (segid 3A4 and resid 130 and name CB) (segid 3A4 and resid 133 and name N)	6.16	0.06	0.05
50	assign (segid 3A4 and resid 130 and name CB) (segid 3A4 and resid 134 and name CA)	6.95	0.11	0.11
	assign (segid 3A4 and resid 130 and name CB) (segid 3A4 and resid 134 and name N)	6.21	0.06	0.05
	assign (segid 3A4 and resid 130 and name CB) (segid 3A4 and resid 135 and name CA)	9.57	0.08	0.08
	assign (segid 3A4 and resid 130 and name CB) (segid 3A4 and resid 135 and name CB)	9.66	0.11	0.11
	assign (segid 3A4 and resid 130 and name CB) (segid 3A4 and resid 136 and name CA)	11.30	0.06	0.07
55	assign (segid 3A4 and resid 130 and name CB) (segid 3A4 and resid 136 and name CB)	11.09	0.23	0.22
	assign (segid 3A4 and resid 130 and name CB) (segid 3A4 and resid 137 and name CA)	11.52	0.17	0.16
	assign (segid 3A4 and resid 130 and name CB) (segid 3A4 and resid 138 and name CA)	12.85	0.28	0.28
	assign (segid 3A4 and resid 130 and name CB) (segid 3A4 and resid 138 and name CB)	12.30	0.36	0.36
	assign (segid 3A4 and resid 130 and name CB) (segid 3A4 and resid 139 and name CA)	14.42	0.87	0.87
60	assign (segid 3A4 and resid 130 and name CB) (segid 3A4 and resid 140 and name CA)	13.34	1.24	1.23
	assign (segid 3A4 and resid 130 and name CB) (segid 3A4 and resid 140 and name CB)	12.69	0.96	0.95
	assign (segid 3A4 and resid 130 and name CB) (segid 3A4 and resid 141 and name CA)	13.63	2.57	2.58
	assign (segid 3A4 and resid 130 and name CB) (segid 3A4 and resid 141 and name CB)	14.79	2.87	2.87
	assign (segid 3A4 and resid 130 and name CB) (segid 3A4 and resid 147 and name CA)	13.68	1.21	1.22
65	assign (segid 3A4 and resid 130 and name CB) (segid 3A4 and resid 147 and name CB)	14.47	1.14	1.14
	assign (segid 3A4 and resid 130 and name CB) (segid 3A4 and resid 148 and name CA)	14.84	2.53	2.52
	assign (segid 3A4 and resid 130 and name CB) (segid 3A4 and resid 149 and name CA)	12.83	3.18	3.17
	assign (segid 3A4 and resid 130 and name CB) (segid 3A4 and resid 149 and name CB)	12.76	3.55	3.54
	assign (segid 3A4 and resid 130 and name CB) (segid 3A4 and resid 150 and name CA)	11.22	1.21	1.22
70	assign (segid 3A4 and resid 130 and name CB) (segid 3A4 and resid 151 and name CA)	12.72	1.24	1.24
	assign (segid 3A4 and resid 130 and name CB) (segid 3A4 and resid 152 and name CA)	13.20	2.57	2.57
	assign (segid 3A4 and resid 130 and name CB) (segid 3A4 and resid 152 and name CB)	13.56	3.36	3.35
	assign (segid 3A4 and resid 130 and name CB) (segid 3A4 and resid 153 and name CA)	11.29	2.11	2.11
	assign (segid 3A4 and resid 130 and name CB) (segid 3A4 and resid 153 and name CB)	10.74	2.12	2.12
75	assign (segid 3A4 and resid 130 and name CB) (segid 3A4 and resid 154 and name CA)	11.20	1.06	1.05
	assign (segid 3A4 and resid 130 and name CB) (segid 3A4 and resid 155 and name CA)	13.69	1.30	1.29
	assign (segid 3A4 and resid 130 and name CB) (segid 3A4 and resid 155 and name CB)	14.45	1.51	1.52
	assign (segid 3A4 and resid 130 and name CB) (segid 3A4 and resid 156 and name CA)	13.67	1.93	1.93
	assign (segid 3A4 and resid 130 and name CB) (segid 3A4 and resid 156 and name CB)	13.34	2.47	2.47
80	assign (segid 3A4 and resid 130 and name CB) (segid 3A4 and resid 157 and name CA)	12.29	1.51	1.51
	assign (segid 3A4 and resid 130 and name CB) (segid 3A4 and resid 157 and name CB)	11.20	1.62	1.63
	assign (segid 3A4 and resid 130 and name CB) (segid 3A4 and resid 158 and name CA)	13.79	1.90	1.89

	assign (segid 3A4 and resid 130 and name CB)	(segid 3A4 and resid 158 and name CB)	13.87	1.97	1.97
	assign (segid 3A4 and resid 130 and name CB)	(segid 3A4 and resid 159 and name CA)	16.44	1.36	1.35
	assign (segid 3A4 and resid 130 and name CB)	(segid 3A4 and resid 159 and name CB)	16.80	1.40	1.40
	assign (segid 3A4 and resid 130 and name CB)	(segid 3A4 and resid 160 and name CA)	16.50	1.51	1.51
	assign (segid 3A4 and resid 130 and name CB)	(segid 3A4 and resid 160 and name CB)	15.85	1.65	1.64
5	assign (segid 3A4 and resid 130 and name CB)	(segid 3A4 and resid 194 and name CB)	15.55	2.11	2.11
	assign (segid 3A4 and resid 130 and name CB)	(segid 3A4 and resid 198 and name CB)	16.87	2.04	2.04
	assign (segid 3A4 and resid 130 and name CB)	(segid 3A4 and resid 219 and name CA)	16.76	0.50	0.50
	assign (segid 3A4 and resid 130 and name CB)	(segid 3A4 and resid 219 and name CB)	16.23	0.72	0.72
	assign (segid 3A4 and resid 130 and name CB)	(segid 3A4 and resid 220 and name CA)	16.20	0.27	0.27
10	assign (segid 3A4 and resid 130 and name CB)	(segid 3A4 and resid 220 and name CB)	14.97	0.26	0.26
	assign (segid 3A4 and resid 130 and name CB)	(segid 3A4 and resid 221 and name CA)	17.66	0.55	0.54
	assign (segid 3A4 and resid 130 and name CB)	(segid 3A4 and resid 221 and name CB)	17.26	0.67	0.67
	assign (segid 3A4 and resid 130 and name CB)	(segid 3A4 and resid 247 and name CA)	17.17	1.02	1.02
	assign (segid 3A4 and resid 130 and name CB)	(segid 3A4 and resid 247 and name CB)	17.87	0.91	0.91
15	assign (segid 3A4 and resid 130 and name CB)	(segid 3A4 and resid 248 and name CA)	14.71	1.39	1.39
	assign (segid 3A4 and resid 130 and name CB)	(segid 3A4 and resid 248 and name CB)	15.24	1.58	1.57
	assign (segid 3A4 and resid 130 and name CB)	(segid 3A4 and resid 249 and name CA)	14.04	1.49	1.49
	assign (segid 3A4 and resid 130 and name CB)	(segid 3A4 and resid 250 and name CB)	13.78	0.69	0.69
	assign (segid 3A4 and resid 130 and name CB)	(segid 3A4 and resid 250 and name CB)	14.94	0.53	0.53
20	assign (segid 3A4 and resid 130 and name CB)	(segid 3A4 and resid 251 and name CA)	11.46	0.52	0.52
	assign (segid 3A4 and resid 130 and name CB)	(segid 3A4 and resid 251 and name CB)	11.88	0.67	0.67
	assign (segid 3A4 and resid 130 and name CB)	(segid 3A4 and resid 252 and name CA)	9.16	1.14	1.15
	assign (segid 3A4 and resid 130 and name CB)	(segid 3A4 and resid 252 and name CB)	9.75	1.58	1.58
	assign (segid 3A4 and resid 130 and name CB)	(segid 3A4 and resid 253 and name CA)	9.94	0.59	0.60
25	assign (segid 3A4 and resid 130 and name CB)	(segid 3A4 and resid 254 and name CA)	10.32	0.64	0.64
	assign (segid 3A4 and resid 130 and name CB)	(segid 3A4 and resid 255 and name CA)	7.67	0.83	0.82
	assign (segid 3A4 and resid 130 and name CB)	(segid 3A4 and resid 256 and name C)	5.75	0.84	0.84
	assign (segid 3A4 and resid 130 and name CB)	(segid 3A4 and resid 256 and name CA)	5.39	0.77	0.77
	assign (segid 3A4 and resid 130 and name CB)	(segid 3A4 and resid 256 and name N)	6.29	0.60	0.60
30	assign (segid 3A4 and resid 130 and name CB)	(segid 3A4 and resid 256 and name O)	5.39	1.09	1.10
	assign (segid 3A4 and resid 130 and name CB)	(segid 3A4 and resid 257 and name CA)	7.60	0.76	0.76
	assign (segid 3A4 and resid 130 and name CB)	(segid 3A4 and resid 257 and name N)	6.83	0.69	0.69
	assign (segid 3A4 and resid 130 and name CB)	(segid 3A4 and resid 258 and name CA)	8.84	1.49	1.48
	assign (segid 3A4 and resid 130 and name CB)	(segid 3A4 and resid 258 and name CB)	9.49	1.47	1.48
35	assign (segid 3A4 and resid 130 and name CB)	(segid 3A4 and resid 259 and name CA)	6.63	2.08	2.08
	assign (segid 3A4 and resid 130 and name CB)	(segid 3A4 and resid 259 and name CB)	5.67	2.18	2.18
	assign (segid 3A4 and resid 130 and name CB)	(segid 3A4 and resid 260 and name CA)	6.40	1.55	1.56
	assign (segid 3A4 and resid 130 and name CB)	(segid 3A4 and resid 260 and name CB)	6.25	1.04	1.04
	assign (segid 3A4 and resid 130 and name CB)	(segid 3A4 and resid 261 and name CA)	9.85	1.40	1.41
40	assign (segid 3A4 and resid 130 and name CB)	(segid 3A4 and resid 262 and name CA)	10.78	1.95	1.95
	assign (segid 3A4 and resid 130 and name CB)	(segid 3A4 and resid 262 and name CB)	10.52	2.07	2.06
	assign (segid 3A4 and resid 130 and name CB)	(segid 3A4 and resid 263 and name CA)	10.04	1.98	1.98
	assign (segid 3A4 and resid 130 and name CB)	(segid 3A4 and resid 263 and name CB)	8.88	1.96	1.96
	assign (segid 3A4 and resid 130 and name CB)	(segid 3A4 and resid 264 and name CA)	11.87	1.43	1.43
45	assign (segid 3A4 and resid 130 and name CB)	(segid 3A4 and resid 265 and name CA)	14.49	1.66	1.66
	assign (segid 3A4 and resid 130 and name CB)	(segid 3A4 and resid 266 and name CA)	15.00	1.98	1.98
	assign (segid 3A4 and resid 130 and name CB)	(segid 3A4 and resid 267 and name CA)	15.74	1.79	1.79
	assign (segid 3A4 and resid 130 and name CB)	(segid 3A4 and resid 267 and name CB)	14.89	1.71	1.72
	assign (segid 3A4 and resid 130 and name CB)	(segid 3A4 and resid 318 and name CA)	14.82	1.67	1.67
50	assign (segid 3A4 and resid 130 and name CB)	(segid 3A4 and resid 318 and name CB)	13.45	1.75	1.74
	assign (segid 3A4 and resid 130 and name CB)	(segid 3A4 and resid 319 and name CA)	16.09	1.58	1.58
	assign (segid 3A4 and resid 130 and name CB)	(segid 3A4 and resid 319 and name CB)	15.67	1.52	1.52
	assign (segid 3A4 and resid 130 and name CB)	(segid 3A4 and resid 391 and name CA)	16.15	1.32	1.31
	assign (segid 3A4 and resid 130 and name CB)	(segid 3A4 and resid 391 and name CB)	15.20	1.44	1.43
55	assign (segid 3A4 and resid 130 and name CB)	(segid 3A4 and resid 392 and name CA)	15.91	1.20	1.21
	assign (segid 3A4 and resid 130 and name CB)	(segid 3A4 and resid 392 and name CB)	16.04	1.07	1.08
	assign (segid 3A4 and resid 130 and name CB)	(segid 3A4 and resid 393 and name CA)	12.57	1.39	1.38
	assign (segid 3A4 and resid 130 and name CB)	(segid 3A4 and resid 394 and name CA)	13.99	1.85	1.85
	assign (segid 3A4 and resid 130 and name CB)	(segid 3A4 and resid 394 and name CB)	15.40	1.88	1.89
60	assign (segid 3A4 and resid 130 and name CB)	(segid 3A4 and resid 395 and name CA)	14.62	1.87	1.86
	assign (segid 3A4 and resid 130 and name CB)	(segid 3A4 and resid 396 and name CA)	11.32	1.82	1.82
	assign (segid 3A4 and resid 130 and name CB)	(segid 3A4 and resid 396 and name CB)	10.76	1.66	1.66
	assign (segid 3A4 and resid 130 and name CB)	(segid 3A4 and resid 397 and name CA)	9.82	2.02	2.03
	assign (segid 3A4 and resid 130 and name CB)	(segid 3A4 and resid 397 and name CB)	10.22	1.95	1.94
65	assign (segid 3A4 and resid 130 and name CB)	(segid 3A4 and resid 398 and name CA)	12.80	2.18	2.18
	assign (segid 3A4 and resid 130 and name CB)	(segid 3A4 and resid 398 and name CB)	14.21	2.15	2.14
	assign (segid 3A4 and resid 130 and name CB)	(segid 3A4 and resid 399 and name CA)	12.63	2.08	2.09
	assign (segid 3A4 and resid 130 and name CB)	(segid 3A4 and resid 399 and name CB)	12.79	1.98	1.98
	assign (segid 3A4 and resid 130 and name CB)	(segid 3A4 and resid 400 and name CA)	9.31	2.09	2.09
70	assign (segid 3A4 and resid 130 and name CB)	(segid 3A4 and resid 400 and name CB)	7.97	2.13	2.14
	assign (segid 3A4 and resid 130 and name CB)	(segid 3A4 and resid 401 and name CA)	10.70	2.18	2.18
	assign (segid 3A4 and resid 130 and name CB)	(segid 3A4 and resid 402 and name CA)	14.05	2.12	2.12
	assign (segid 3A4 and resid 130 and name CB)	(segid 3A4 and resid 402 and name CB)	14.94	2.17	2.18
	assign (segid 3A4 and resid 130 and name CB)	(segid 3A4 and resid 403 and name CA)	13.34	1.90	1.90
75	assign (segid 3A4 and resid 130 and name CB)	(segid 3A4 and resid 403 and name CB)	12.71	1.88	1.88
	assign (segid 3A4 and resid 130 and name CB)	(segid 3A4 and resid 404 and name CA)	11.57	1.65	1.65
	assign (segid 3A4 and resid 130 and name CB)	(segid 3A4 and resid 404 and name CB)	10.31	1.62	1.61
	assign (segid 3A4 and resid 130 and name CB)	(segid 3A4 and resid 405 and name CA)	14.32	1.55	1.55
	assign (segid 3A4 and resid 130 and name CB)	(segid 3A4 and resid 405 and name CB)	14.65	1.65	1.65
80	assign (segid 3A4 and resid 130 and name CB)	(segid 3A4 and resid 407 and name CA)	16.32	1.48	1.47
	assign (segid 3A4 and resid 130 and name CB)	(segid 3A4 and resid 407 and name CB)	15.35	1.47	1.48
	assign (segid 3A4 and resid 130 and name CB)	(segid 3A4 and resid 408 and name CA)	15.94	1.37	1.36

	assign (segid 3A4 and resid 130 and name CB)	(segid 3A4 and resid 408 and name CB)	15.05	1.42	1.41
	assign (segid 3A4 and resid 130 and name CB)	(segid 3A4 and resid 431 and name CA)	17.82	1.11	1.11
	assign (segid 3A4 and resid 130 and name CB)	(segid 3A4 and resid 433 and name CA)	15.86	1.40	1.40
	assign (segid 3A4 and resid 130 and name CB)	(segid 3A4 and resid 434 and name CA)	14.26	1.32	1.31
	assign (segid 3A4 and resid 130 and name CB)	(segid 3A4 and resid 435 and name CA)	15.23	1.78	1.77
5	assign (segid 3A4 and resid 130 and name N)	(segid 3A4 and resid 130 and name C)	2.50	0.03	0.03
	assign (segid 3A4 and resid 130 and name N)	(segid 3A4 and resid 130 and name CA)	1.47	0.01	0.02
	assign (segid 3A4 and resid 130 and name N)	(segid 3A4 and resid 130 and name CB)	2.39	0.04	0.04
	assign (segid 3A4 and resid 130 and name N)	(segid 3A4 and resid 130 and name O)	3.57	0.04	0.03
	assign (segid 3A4 and resid 130 and name N)	(segid 3A4 and resid 131 and name C)	4.78	0.08	0.07
10	assign (segid 3A4 and resid 130 and name N)	(segid 3A4 and resid 131 and name CA)	4.22	0.04	0.04
	assign (segid 3A4 and resid 130 and name N)	(segid 3A4 and resid 131 and name CB)	5.01	0.07	0.06
	assign (segid 3A4 and resid 130 and name N)	(segid 3A4 and resid 131 and name N)	2.81	0.03	0.04
	assign (segid 3A4 and resid 130 and name N)	(segid 3A4 and resid 131 and name O)	5.86	0.06	0.05
	assign (segid 3A4 and resid 130 and name N)	(segid 3A4 and resid 132 and name C)	5.86	0.09	0.09
15	assign (segid 3A4 and resid 130 and name N)	(segid 3A4 and resid 132 and name CA)	5.54	0.14	0.14
	assign (segid 3A4 and resid 130 and name N)	(segid 3A4 and resid 132 and name CB)	5.68	0.19	0.18
	assign (segid 3A4 and resid 130 and name N)	(segid 3A4 and resid 132 and name N)	4.48	0.15	0.14
	assign (segid 3A4 and resid 130 and name N)	(segid 3A4 and resid 132 and name O)	7.07	0.09	0.09
	assign (segid 3A4 and resid 130 and name N)	(segid 3A4 and resid 133 and name C)	6.62	0.07	0.08
20	assign (segid 3A4 and resid 130 and name N)	(segid 3A4 and resid 133 and name CA)	5.85	0.10	0.10
	assign (segid 3A4 and resid 130 and name N)	(segid 3A4 and resid 133 and name CB)	5.32	0.20	0.19
	assign (segid 3A4 and resid 130 and name N)	(segid 3A4 and resid 133 and name CG1)	5.25	0.27	0.27
	assign (segid 3A4 and resid 130 and name N)	(segid 3A4 and resid 133 and name CG2)	6.54	0.23	0.23
	assign (segid 3A4 and resid 130 and name N)	(segid 3A4 and resid 133 and name N)	5.06	0.07	0.07
25	assign (segid 3A4 and resid 130 and name N)	(segid 3A4 and resid 133 and name O)	7.83	0.07	0.06
	assign (segid 3A4 and resid 130 and name N)	(segid 3A4 and resid 134 and name CA)	7.29	0.12	0.12
	assign (segid 3A4 and resid 130 and name N)	(segid 3A4 and resid 134 and name N)	6.18	0.09	0.09
	assign (segid 3A4 and resid 130 and name N)	(segid 3A4 and resid 259 and name CB)	6.35	0.61	0.62
	assign (segid 3A4 and resid 130 and name N)	(segid 3A4 and resid 260 and name CA)	6.70	0.47	0.46
30	assign (segid 3A4 and resid 130 and name N)	(segid 3A4 and resid 260 and name CB)	6.60	0.23	0.23
	assign (segid 3A4 and resid 130 and name N)	(segid 3A4 and resid 260 and name N)	6.56	0.46	0.47
	assign (segid 3A4 and resid 130 and name N)	(segid 3A4 and resid 130 and name CB)	3.30	0.02	0.01
	assign (segid 3A4 and resid 130 and name O)	(segid 3A4 and resid 131 and name C)	3.02	0.06	0.05
	assign (segid 3A4 and resid 130 and name O)	(segid 3A4 and resid 131 and name CA)	2.73	0.04	0.05
35	assign (segid 3A4 and resid 130 and name O)	(segid 3A4 and resid 131 and name CB)	4.22	0.04	0.04
	assign (segid 3A4 and resid 130 and name O)	(segid 3A4 and resid 131 and name N)	2.25	0.02	0.01
	assign (segid 3A4 and resid 130 and name O)	(segid 3A4 and resid 131 and name O)	3.47	0.09	0.08
	assign (segid 3A4 and resid 130 and name O)	(segid 3A4 and resid 132 and name C)	4.29	0.08	0.08
	assign (segid 3A4 and resid 130 and name O)	(segid 3A4 and resid 132 and name CA)	4.56	0.08	0.07
40	assign (segid 3A4 and resid 130 and name O)	(segid 3A4 and resid 132 and name CB)	5.57	0.10	0.09
	assign (segid 3A4 and resid 130 and name O)	(segid 3A4 and resid 132 and name N)	3.59	0.07	0.08
	assign (segid 3A4 and resid 130 and name O)	(segid 3A4 and resid 132 and name O)	5.21	0.11	0.10
	assign (segid 3A4 and resid 130 and name O)	(segid 3A4 and resid 133 and name C)	3.91	0.06	0.07
	assign (segid 3A4 and resid 130 and name O)	(segid 3A4 and resid 133 and name CA)	3.93	0.06	0.06
45	assign (segid 3A4 and resid 130 and name O)	(segid 3A4 and resid 133 and name CB)	3.87	0.12	0.11
	assign (segid 3A4 and resid 130 and name O)	(segid 3A4 and resid 133 and name CG1)	4.83	0.14	0.14
	assign (segid 3A4 and resid 130 and name O)	(segid 3A4 and resid 133 and name CG2)	4.84	0.13	0.14
	assign (segid 3A4 and resid 130 and name O)	(segid 3A4 and resid 133 and name N)	3.49	0.04	0.04
	assign (segid 3A4 and resid 130 and name O)	(segid 3A4 and resid 133 and name O)	5.07	0.09	0.08
50	assign (segid 3A4 and resid 130 and name O)	(segid 3A4 and resid 134 and name C)	4.98	0.07	0.06
	assign (segid 3A4 and resid 130 and name O)	(segid 3A4 and resid 134 and name CA)	3.84	0.10	0.10
	assign (segid 3A4 and resid 130 and name O)	(segid 3A4 and resid 134 and name N)	3.01	0.07	0.08
	assign (segid 3A4 and resid 130 and name O)	(segid 3A4 and resid 134 and name O)	6.12	0.08	0.08
	assign (segid 3A4 and resid 130 and name O)	(segid 3A4 and resid 135 and name C)	7.24	0.07	0.07
55	assign (segid 3A4 and resid 130 and name O)	(segid 3A4 and resid 135 and name CA)	6.34	0.09	0.10
	assign (segid 3A4 and resid 130 and name O)	(segid 3A4 and resid 135 and name CB)	6.59	0.14	0.14
	assign (segid 3A4 and resid 130 and name O)	(segid 3A4 and resid 135 and name N)	4.99	0.08	0.07
	assign (segid 3A4 and resid 130 and name O)	(segid 3A4 and resid 136 and name N)	6.97	0.06	0.06
	assign (segid 3A4 and resid 130 and name O)	(segid 3A4 and resid 137 and name N)	7.75	0.10	0.10
60	assign (segid 3A4 and resid 130 and name O)	(segid 3A4 and resid 256 and name CA)	6.02	0.77	0.78
	assign (segid 3A4 and resid 130 and name O)	(segid 3A4 and resid 256 and name N)	6.52	0.77	0.78
	assign (segid 3A4 and resid 131 and name C)	(segid 3A4 and resid 131 and name CB)	2.51	0.02	0.03
	assign (segid 3A4 and resid 131 and name C)	(segid 3A4 and resid 131 and name O)	1.24	0.01	0.01
65	assign (segid 3A4 and resid 131 and name C)	(segid 3A4 and resid 132 and name C)	2.99	0.05	0.06
	assign (segid 3A4 and resid 131 and name C)	(segid 3A4 and resid 132 and name CA)	2.42	0.01	0.01
	assign (segid 3A4 and resid 131 and name C)	(segid 3A4 and resid 132 and name CB)	3.71	0.02	0.03
	assign (segid 3A4 and resid 131 and name C)	(segid 3A4 and resid 132 and name N)	1.33	0.00	0.01
	assign (segid 3A4 and resid 131 and name C)	(segid 3A4 and resid 132 and name O)	3.86	0.09	0.09
70	assign (segid 3A4 and resid 131 and name C)	(segid 3A4 and resid 133 and name C)	4.49	0.07	0.07
	assign (segid 3A4 and resid 131 and name C)	(segid 3A4 and resid 133 and name CA)	4.42	0.06	0.06
	assign (segid 3A4 and resid 131 and name C)	(segid 3A4 and resid 133 and name CB)	5.23	0.08	0.08
	assign (segid 3A4 and resid 131 and name C)	(segid 3A4 and resid 133 and name CG1)	5.90	0.08	0.08
	assign (segid 3A4 and resid 131 and name C)	(segid 3A4 and resid 133 and name CG2)	6.50	0.08	0.09
	assign (segid 3A4 and resid 131 and name C)	(segid 3A4 and resid 133 and name N)	3.25	0.06	0.05
75	assign (segid 3A4 and resid 131 and name C)	(segid 3A4 and resid 133 and name O)	5.54	0.05	0.05
	assign (segid 3A4 and resid 131 and name C)	(segid 3A4 and resid 134 and name C)	4.81	0.15	0.15
	assign (segid 3A4 and resid 131 and name C)	(segid 3A4 and resid 134 and name CA)	4.55	0.20	0.20
	assign (segid 3A4 and resid 131 and name C)	(segid 3A4 and resid 134 and name N)	3.80	0.16	0.17
80	assign (segid 3A4 and resid 131 and name C)	(segid 3A4 and resid 134 and name O)	6.02	0.14	0.14
	assign (segid 3A4 and resid 131 and name C)	(segid 3A4 and resid 135 and name C)	5.98	0.07	0.06
	assign (segid 3A4 and resid 131 and name C)	(segid 3A4 and resid 135 and name CA)	4.91	0.10	0.10
	assign (segid 3A4 and resid 131 and name C)	(segid 3A4 and resid 135 and name CB)	4.50	0.11	0.10

	assign (segid 3A4 and resid 131 and name C) (segid 3A4 and resid 135 and name N)	4.04	0.12	0.11
	assign (segid 3A4 and resid 131 and name C) (segid 3A4 and resid 135 and name O)	7.14	0.07	0.08
	assign (segid 3A4 and resid 131 and name C) (segid 3A4 and resid 136 and name CA)	7.16	0.10	0.11
	assign (segid 3A4 and resid 131 and name C) (segid 3A4 and resid 136 and name CB)	7.24	0.20	0.19
5	assign (segid 3A4 and resid 131 and name C) (segid 3A4 and resid 136 and name N)	5.87	0.09	0.08
	assign (segid 3A4 and resid 131 and name C) (segid 3A4 and resid 137 and name N)	7.66	0.09	0.09
	assign (segid 3A4 and resid 131 and name CA) (segid 3A4 and resid 131 and name C)	1.52	0.00	0.01
	assign (segid 3A4 and resid 131 and name CA) (segid 3A4 and resid 131 and name CB)	1.53	0.02	0.02
	assign (segid 3A4 and resid 131 and name CA) (segid 3A4 and resid 131 and name O)	2.40	0.02	0.02
10	assign (segid 3A4 and resid 131 and name CA) (segid 3A4 and resid 132 and name C)	4.40	0.06	0.06
	assign (segid 3A4 and resid 131 and name CA) (segid 3A4 and resid 132 and name CA)	3.81	0.02	0.03
	assign (segid 3A4 and resid 131 and name CA) (segid 3A4 and resid 132 and name CB)	4.89	0.01	0.02
	assign (segid 3A4 and resid 131 and name CA) (segid 3A4 and resid 132 and name N)	2.45	0.03	0.03
	assign (segid 3A4 and resid 131 and name CA) (segid 3A4 and resid 132 and name O)	5.33	0.10	0.09
	assign (segid 3A4 and resid 131 and name CA) (segid 3A4 and resid 133 and name C)	5.44	0.10	0.09
15	assign (segid 3A4 and resid 131 and name CA) (segid 3A4 and resid 133 and name CA)	5.43	0.06	0.06
	assign (segid 3A4 and resid 131 and name CA) (segid 3A4 and resid 133 and name CB)	5.92	0.10	0.10
	assign (segid 3A4 and resid 131 and name CA) (segid 3A4 and resid 133 and name CG1)	6.61	0.13	0.13
	assign (segid 3A4 and resid 131 and name CA) (segid 3A4 and resid 133 and name CG2)	7.14	0.10	0.10
20	assign (segid 3A4 and resid 131 and name CA) (segid 3A4 and resid 133 and name N)	4.36	0.05	0.06
	assign (segid 3A4 and resid 131 and name CA) (segid 3A4 and resid 133 and name O)	6.54	0.10	0.09
	assign (segid 3A4 and resid 131 and name CA) (segid 3A4 and resid 134 and name C)	5.61	0.18	0.17
	assign (segid 3A4 and resid 131 and name CA) (segid 3A4 and resid 134 and name CA)	5.10	0.25	0.24
	assign (segid 3A4 and resid 131 and name CA) (segid 3A4 and resid 134 and name N)	4.52	0.18	0.17
	assign (segid 3A4 and resid 131 and name CA) (segid 3A4 and resid 134 and name O)	6.80	0.18	0.18
25	assign (segid 3A4 and resid 131 and name CA) (segid 3A4 and resid 135 and name C)	7.21	0.07	0.07
	assign (segid 3A4 and resid 131 and name CA) (segid 3A4 and resid 135 and name CA)	6.01	0.09	0.09
	assign (segid 3A4 and resid 131 and name CA) (segid 3A4 and resid 135 and name CB)	5.66	0.09	0.09
	assign (segid 3A4 and resid 131 and name CA) (segid 3A4 and resid 135 and name N)	5.05	0.12	0.11
	assign (segid 3A4 and resid 131 and name CA) (segid 3A4 and resid 136 and name CA)	8.53	0.08	0.09
30	assign (segid 3A4 and resid 131 and name CA) (segid 3A4 and resid 136 and name CB)	8.65	0.18	0.18
	assign (segid 3A4 and resid 131 and name CA) (segid 3A4 and resid 136 and name N)	7.21	0.08	0.07
	assign (segid 3A4 and resid 131 and name CA) (segid 3A4 and resid 137 and name CA)	9.75	0.15	0.15
	assign (segid 3A4 and resid 131 and name CA) (segid 3A4 and resid 138 and name CA)	10.40	0.23	0.23
	assign (segid 3A4 and resid 131 and name CA) (segid 3A4 and resid 138 and name CB)	9.84	0.48	0.47
35	assign (segid 3A4 and resid 131 and name CA) (segid 3A4 and resid 139 and name CA)	11.16	0.88	0.88
	assign (segid 3A4 and resid 131 and name CA) (segid 3A4 and resid 140 and name CA)	9.66	0.88	0.87
	assign (segid 3A4 and resid 131 and name CA) (segid 3A4 and resid 140 and name CB)	9.12	0.41	0.42
	assign (segid 3A4 and resid 131 and name CA) (segid 3A4 and resid 141 and name CA)	9.70	2.28	2.28
	assign (segid 3A4 and resid 131 and name CA) (segid 3A4 and resid 141 and name CB)	10.72	2.68	2.68
40	assign (segid 3A4 and resid 131 and name CA) (segid 3A4 and resid 147 and name CA)	11.41	1.43	1.43
	assign (segid 3A4 and resid 131 and name CA) (segid 3A4 and resid 147 and name CB)	12.28	1.76	1.77
	assign (segid 3A4 and resid 131 and name CA) (segid 3A4 and resid 148 and name CA)	12.46	0.55	0.55
	assign (segid 3A4 and resid 131 and name CA) (segid 3A4 and resid 149 and name CA)	10.56	0.72	0.71
	assign (segid 3A4 and resid 131 and name CA) (segid 3A4 and resid 149 and name CB)	10.38	1.13	1.14
45	assign (segid 3A4 and resid 131 and name CA) (segid 3A4 and resid 150 and name CA)	9.28	1.75	1.75
	assign (segid 3A4 and resid 131 and name CA) (segid 3A4 and resid 151 and name CA)	11.14	1.95	1.95
	assign (segid 3A4 and resid 131 and name CA) (segid 3A4 and resid 152 and name CA)	11.65	0.86	0.85
	assign (segid 3A4 and resid 131 and name CA) (segid 3A4 and resid 152 and name CB)	11.81	0.99	0.99
	assign (segid 3A4 and resid 131 and name CA) (segid 3A4 and resid 153 and name CA)	10.12	1.63	1.63
50	assign (segid 3A4 and resid 131 and name CA) (segid 3A4 and resid 153 and name CB)	9.48	1.71	1.70
	assign (segid 3A4 and resid 131 and name CA) (segid 3A4 and resid 154 and name CA)	10.44	3.27	3.26
	assign (segid 3A4 and resid 131 and name CA) (segid 3A4 and resid 155 and name CA)	13.14	2.37	2.37
	assign (segid 3A4 and resid 131 and name CA) (segid 3A4 and resid 155 and name CB)	13.70	1.86	1.86
	assign (segid 3A4 and resid 131 and name CA) (segid 3A4 and resid 156 and name CA)	13.22	1.92	1.93
55	assign (segid 3A4 and resid 131 and name CA) (segid 3A4 and resid 156 and name CB)	12.72	1.70	1.70
	assign (segid 3A4 and resid 131 and name CA) (segid 3A4 and resid 157 and name CA)	12.49	3.08	3.07
	assign (segid 3A4 and resid 131 and name CA) (segid 3A4 and resid 157 and name CB)	11.40	3.43	3.44
	assign (segid 3A4 and resid 131 and name CA) (segid 3A4 and resid 190 and name CB)	17.74	1.44	1.45
60	assign (segid 3A4 and resid 131 and name CA) (segid 3A4 and resid 191 and name CA)	18.28	1.18	1.19
	assign (segid 3A4 and resid 131 and name CA) (segid 3A4 and resid 193 and name CA)	17.79	1.07	1.06
	assign (segid 3A4 and resid 131 and name CA) (segid 3A4 and resid 193 and name CB)	17.42	1.19	1.19
	assign (segid 3A4 and resid 131 and name CA) (segid 3A4 and resid 194 and name CA)	14.95	0.96	0.95
	assign (segid 3A4 and resid 131 and name CA) (segid 3A4 and resid 194 and name CB)	14.42	1.06	1.05
65	assign (segid 3A4 and resid 131 and name CA) (segid 3A4 and resid 195 and name CA)	17.54	0.86	0.87
	assign (segid 3A4 and resid 131 and name CA) (segid 3A4 and resid 195 and name CB)	18.79	0.87	0.87
	assign (segid 3A4 and resid 131 and name CA) (segid 3A4 and resid 197 and name CA)	15.62	0.96	0.97
	assign (segid 3A4 and resid 131 and name CA) (segid 3A4 and resid 197 and name CB)	14.39	0.95	0.96
	assign (segid 3A4 and resid 131 and name CA) (segid 3A4 and resid 198 and name CA)	15.17	0.89	0.88
70	assign (segid 3A4 and resid 131 and name CA) (segid 3A4 and resid 198 and name CB)	14.98	0.74	0.73
	assign (segid 3A4 and resid 131 and name CA) (segid 3A4 and resid 201 and name CA)	16.46	1.16	1.16
	assign (segid 3A4 and resid 131 and name CA) (segid 3A4 and resid 201 and name CB)	15.00	1.12	1.12
	assign (segid 3A4 and resid 131 and name CA) (segid 3A4 and resid 202 and name CA)	18.55	0.94	0.94
	assign (segid 3A4 and resid 131 and name CA) (segid 3A4 and resid 205 and name CB)	18.52	1.00	1.00
75	assign (segid 3A4 and resid 131 and name CA) (segid 3A4 and resid 219 and name CA)	14.44	0.74	0.73
	assign (segid 3A4 and resid 131 and name CA) (segid 3A4 and resid 219 and name CB)	13.66	0.83	0.84
	assign (segid 3A4 and resid 131 and name CA) (segid 3A4 and resid 220 and name CA)	14.48	0.33	0.32
	assign (segid 3A4 and resid 131 and name CA) (segid 3A4 and resid 220 and name CB)	13.47	0.30	0.31
	assign (segid 3A4 and resid 131 and name CA) (segid 3A4 and resid 221 and name CA)	15.54	0.26	0.26
	assign (segid 3A4 and resid 131 and name CA) (segid 3A4 and resid 221 and name CB)	14.92	0.27	0.28
80	assign (segid 3A4 and resid 131 and name CA) (segid 3A4 and resid 222 and name CA)	18.36	0.46	0.45
	assign (segid 3A4 and resid 131 and name CA) (segid 3A4 and resid 222 and name CB)	18.41	0.56	0.55
	assign (segid 3A4 and resid 131 and name CA) (segid 3A4 and resid 223 and name CB)	18.81	0.35	0.35

	assign (segid 3A4 and resid 131 and name CA)	(segid 3A4 and resid 224 and name CB)	18.64	0.33	0.34
	assign (segid 3A4 and resid 131 and name CA)	(segid 3A4 and resid 245 and name CA)	17.95	0.74	0.74
	assign (segid 3A4 and resid 131 and name CA)	(segid 3A4 and resid 246 and name CA)	18.18	0.61	0.61
	assign (segid 3A4 and resid 131 and name CA)	(segid 3A4 and resid 247 and name CA)	16.67	0.50	0.50
5	assign (segid 3A4 and resid 131 and name CA)	(segid 3A4 and resid 247 and name CB)	17.28	0.43	0.44
	assign (segid 3A4 and resid 131 and name CA)	(segid 3A4 and resid 248 and name CA)	13.63	0.62	0.61
	assign (segid 3A4 and resid 131 and name CA)	(segid 3A4 and resid 248 and name CB)	13.83	0.73	0.73
	assign (segid 3A4 and resid 131 and name CA)	(segid 3A4 and resid 249 and name CA)	13.39	0.63	0.62
	assign (segid 3A4 and resid 131 and name CA)	(segid 3A4 and resid 250 and name CA)	13.94	0.57	0.58
10	assign (segid 3A4 and resid 131 and name CA)	(segid 3A4 and resid 250 and name CB)	15.21	0.56	0.56
	assign (segid 3A4 and resid 131 and name CA)	(segid 3A4 and resid 251 and name CA)	11.42	0.44	0.45
	assign (segid 3A4 and resid 131 and name CA)	(segid 3A4 and resid 251 and name CB)	11.52	0.36	0.37
	assign (segid 3A4 and resid 131 and name CA)	(segid 3A4 and resid 252 and name CA)	8.74	0.67	0.68
	assign (segid 3A4 and resid 131 and name CA)	(segid 3A4 and resid 252 and name CB)	8.99	0.71	0.70
15	assign (segid 3A4 and resid 131 and name CA)	(segid 3A4 and resid 253 and name CA)	10.49	1.15	1.15
	assign (segid 3A4 and resid 131 and name CA)	(segid 3A4 and resid 254 and name CA)	11.68	1.26	1.27
	assign (segid 3A4 and resid 131 and name CA)	(segid 3A4 and resid 255 and name CA)	8.93	1.37	1.36
	assign (segid 3A4 and resid 131 and name CA)	(segid 3A4 and resid 256 and name CA)	6.79	1.21	1.21
	assign (segid 3A4 and resid 131 and name CA)	(segid 3A4 and resid 257 and name CA)	9.75	1.34	1.33
20	assign (segid 3A4 and resid 131 and name CA)	(segid 3A4 and resid 258 and name CA)	11.72	1.38	1.38
	assign (segid 3A4 and resid 131 and name CA)	(segid 3A4 and resid 258 and name CB)	12.28	1.32	1.33
	assign (segid 3A4 and resid 131 and name CA)	(segid 3A4 and resid 259 and name CA)	9.91	1.16	1.16
	assign (segid 3A4 and resid 131 and name CA)	(segid 3A4 and resid 259 and name CB)	8.88	1.09	1.08
	assign (segid 3A4 and resid 131 and name CA)	(segid 3A4 and resid 260 and name CA)	9.32	1.17	1.18
25	assign (segid 3A4 and resid 131 and name CA)	(segid 3A4 and resid 260 and name CB)	8.76	1.11	1.12
	assign (segid 3A4 and resid 131 and name CA)	(segid 3A4 and resid 261 and name CA)	12.97	1.19	1.19
	assign (segid 3A4 and resid 131 and name CA)	(segid 3A4 and resid 262 and name CA)	14.17	1.06	1.06
	assign (segid 3A4 and resid 131 and name CA)	(segid 3A4 and resid 262 and name CB)	13.92	1.03	1.03
	assign (segid 3A4 and resid 131 and name CA)	(segid 3A4 and resid 263 and name CA)	13.14	0.87	0.88
30	assign (segid 3A4 and resid 131 and name CA)	(segid 3A4 and resid 263 and name CB)	11.83	0.82	0.82
	assign (segid 3A4 and resid 131 and name CA)	(segid 3A4 and resid 264 and name CA)	14.78	0.85	0.86
	assign (segid 3A4 and resid 131 and name CA)	(segid 3A4 and resid 265 and name CA)	17.70	0.95	0.95
	assign (segid 3A4 and resid 131 and name CA)	(segid 3A4 and resid 267 and name CA)	18.52	0.81	0.82
	assign (segid 3A4 and resid 131 and name CA)	(segid 3A4 and resid 267 and name CB)	17.53	0.83	0.83
35	assign (segid 3A4 and resid 131 and name CA)	(segid 3A4 and resid 318 and name CB)	16.61	1.39	1.40
	assign (segid 3A4 and resid 131 and name CA)	(segid 3A4 and resid 391 and name CA)	18.16	0.83	0.84
	assign (segid 3A4 and resid 131 and name CA)	(segid 3A4 and resid 391 and name CB)	17.40	0.86	0.86
	assign (segid 3A4 and resid 131 and name CA)	(segid 3A4 and resid 392 and name CA)	17.30	0.75	0.75
	assign (segid 3A4 and resid 131 and name CA)	(segid 3A4 and resid 392 and name CB)	17.18	0.79	0.78
40	assign (segid 3A4 and resid 131 and name CA)	(segid 3A4 and resid 393 and name CA)	14.06	0.70	0.71
	assign (segid 3A4 and resid 131 and name CA)	(segid 3A4 and resid 394 and name CA)	16.14	0.78	0.77
	assign (segid 3A4 and resid 131 and name CA)	(segid 3A4 and resid 394 and name CB)	17.61	0.81	0.80
	assign (segid 3A4 and resid 131 and name CA)	(segid 3A4 and resid 395 and name CA)	16.33	0.51	0.51
	assign (segid 3A4 and resid 131 and name CA)	(segid 3A4 and resid 396 and name CA)	12.69	0.47	0.46
45	assign (segid 3A4 and resid 131 and name CA)	(segid 3A4 and resid 396 and name CB)	11.83	0.50	0.50
	assign (segid 3A4 and resid 131 and name CA)	(segid 3A4 and resid 397 and name CA)	12.21	0.60	0.60
	assign (segid 3A4 and resid 131 and name CA)	(segid 3A4 and resid 397 and name CB)	12.79	0.68	0.67
	assign (segid 3A4 and resid 131 and name CA)	(segid 3A4 and resid 398 and name CA)	15.25	0.50	0.50
	assign (segid 3A4 and resid 131 and name CA)	(segid 3A4 and resid 398 and name CB)	16.62	0.50	0.50
50	assign (segid 3A4 and resid 131 and name CA)	(segid 3A4 and resid 399 and name CA)	14.37	0.37	0.36
	assign (segid 3A4 and resid 131 and name CA)	(segid 3A4 and resid 399 and name CB)	14.18	0.41	0.41
	assign (segid 3A4 and resid 131 and name CA)	(segid 3A4 and resid 400 and name CA)	11.18	0.30	0.30
	assign (segid 3A4 and resid 131 and name CA)	(segid 3A4 and resid 400 and name CB)	9.94	0.41	0.42
	assign (segid 3A4 and resid 131 and name CA)	(segid 3A4 and resid 401 and name CA)	13.33	0.47	0.47
55	assign (segid 3A4 and resid 131 and name CA)	(segid 3A4 and resid 402 and name CA)	16.26	0.27	0.27
	assign (segid 3A4 and resid 131 and name CA)	(segid 3A4 and resid 402 and name CB)	17.07	0.30	0.30
	assign (segid 3A4 and resid 131 and name CA)	(segid 3A4 and resid 403 and name CA)	14.80	0.17	0.16
	assign (segid 3A4 and resid 131 and name CA)	(segid 3A4 and resid 403 and name CB)	13.88	0.16	0.17
	assign (segid 3A4 and resid 131 and name CA)	(segid 3A4 and resid 404 and name CA)	13.27	0.34	0.34
60	assign (segid 3A4 and resid 131 and name CA)	(segid 3A4 and resid 404 and name CB)	12.24	0.36	0.35
	assign (segid 3A4 and resid 131 and name CA)	(segid 3A4 and resid 405 and name CA)	16.54	0.42	0.41
	assign (segid 3A4 and resid 131 and name CA)	(segid 3A4 and resid 405 and name CB)	17.10	0.38	0.37
	assign (segid 3A4 and resid 131 and name CA)	(segid 3A4 and resid 406 and name CA)	18.75	0.34	0.35
	assign (segid 3A4 and resid 131 and name CA)	(segid 3A4 and resid 407 and name CA)	17.46	0.40	0.39
65	assign (segid 3A4 and resid 131 and name CA)	(segid 3A4 and resid 407 and name CB)	16.26	0.41	0.41
	assign (segid 3A4 and resid 131 and name CA)	(segid 3A4 and resid 408 and name CA)	17.39	0.28	0.29
	assign (segid 3A4 and resid 131 and name CA)	(segid 3A4 and resid 408 and name CB)	16.73	0.27	0.28
	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 132 and name C)	5.44	0.05	0.05
70	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 132 and name CA)	4.51	0.04	0.04
	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 132 and name CB)	5.41	0.07	0.08
	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 132 and name N)	3.19	0.05	0.05
	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 132 and name O)	6.31	0.10	0.10
	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 133 and name C)	6.84	0.10	0.10
	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 133 and name CA)	6.81	0.08	0.07
75	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 133 and name CB)	7.36	0.12	0.12
	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 133 and name N)	5.62	0.07	0.08
	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 134 and name C)	6.72	0.22	0.21
	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 134 and name CA)	6.41	0.29	0.28
	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 134 and name N)	5.94	0.19	0.19
80	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 135 and name CA)	6.73	0.13	0.12
	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 135 and name CB)	6.09	0.08	0.09
	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 135 and name N)	6.01	0.16	0.16
	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 136 and name CA)	9.50	0.10	0.11

	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 136 and name CB)	9.68	0.18	0.18
	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 137 and name CA)	10.98	0.15	0.16
	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 138 and name CA)	11.33	0.28	0.28
	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 138 and name CB)	10.70	0.58	0.58
	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 139 and name CA)	11.80	0.94	0.94
5	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 140 and name CA)	9.94	0.88	0.87
	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 140 and name CB)	9.38	0.35	0.35
	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 141 and name CA)	9.62	2.39	2.40
	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 141 and name CB)	10.49	2.87	2.87
	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 147 and name CA)	11.25	1.57	1.57
10	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 147 and name CB)	12.15	1.87	1.86
	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 148 and name CA)	12.19	0.62	0.62
	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 149 and name CB)	10.22	0.53	0.54
	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 149 and name CA)	10.09	0.92	0.91
	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 150 and name CA)	8.78	2.21	2.20
15	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 151 and name CA)	10.47	2.62	2.63
	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 152 and name CA)	11.15	1.35	1.35
	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 152 and name CB)	11.39	0.83	0.82
	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 153 and name CA)	9.72	2.14	2.14
	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 153 and name CB)	9.14	2.13	2.12
20	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 154 and name CA)	9.78	3.98	3.99
	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 155 and name CA)	12.56	3.16	3.17
	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 155 and name CB)	13.12	2.64	2.65
	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 156 and name CA)	12.88	2.51	2.51
	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 156 and name CB)	12.45	2.10	2.10
25	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 190 and name CB)	17.45	1.85	1.84
	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 193 and name CA)	17.60	1.08	1.07
	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 193 and name CB)	17.14	1.19	1.18
	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 194 and name CA)	14.96	1.09	1.10
	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 194 and name CB)	14.48	1.34	1.34
30	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 195 and name CA)	17.75	0.96	0.96
	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 197 and name CA)	15.66	0.69	0.70
	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 197 and name CB)	14.39	0.69	0.69
	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 198 and name CA)	15.52	0.59	0.59
	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 198 and name CB)	15.40	0.51	0.50
35	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 201 and name CA)	16.84	0.96	0.96
	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 201 and name CB)	15.40	0.91	0.92
	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 219 and name CA)	15.43	0.79	0.79
	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 219 and name CB)	14.59	0.87	0.86
	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 220 and name CA)	15.59	0.35	0.34
40	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 220 and name CB)	14.63	0.34	0.34
	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 221 and name CA)	16.46	0.25	0.24
	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 221 and name CB)	15.76	0.26	0.26
	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 222 and name CA)	19.25	0.42	0.41
	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 222 and name CB)	18.61	0.54	0.55
45	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 245 and name CA)	18.89	0.68	0.67
	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 246 and name CA)	17.57	0.50	0.51
	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 247 and name CA)	18.25	0.38	0.38
	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 248 and name CA)	14.48	0.49	0.49
	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 248 and name CB)	14.62	0.56	0.56
50	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 249 and name CA)	14.02	0.79	0.80
	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 249 and name CB)	14.73	0.92	0.93
	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 250 and name CA)	16.05	0.90	0.90
	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 250 and name CB)	12.44	0.67	0.66
	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 251 and name CA)	12.60	0.44	0.44
55	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 251 and name CB)	9.54	0.94	0.94
	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 252 and name CA)	9.66	0.92	0.91
	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 252 and name CB)	11.03	1.60	1.59
	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 253 and name CA)	12.47	1.57	1.58
	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 254 and name CA)	9.88	1.52	1.52
60	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 255 and name CA)	7.37	1.53	1.52
	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 256 and name CA)	9.98	1.69	1.69
	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 257 and name CA)	12.23	1.58	1.59
	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 258 and name CA)	12.92	1.51	1.52
	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 259 and name CA)	10.54	1.19	1.18
65	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 259 and name CB)	9.64	1.05	1.06
	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 260 and name CA)	9.46	1.30	1.31
	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 260 and name CB)	8.75	1.34	1.33
	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 261 and name CA)	13.07	1.37	1.37
	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 262 and name CA)	14.51	1.07	1.07
70	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 262 and name CB)	14.39	1.01	1.01
	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 263 and name CA)	13.34	0.78	0.78
	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 263 and name CB)	12.01	0.70	0.71
	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 264 and name CA)	14.69	0.87	0.86
	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 265 and name CA)	17.74	0.97	0.97
75	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 266 and name CA)	18.32	0.74	0.74
	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 267 and name CA)	18.46	0.68	0.68
	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 267 and name CB)	17.40	0.69	0.69
	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 267 and name CA)	15.30	0.71	0.70
	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 267 and name CB)	17.28	0.71	0.71
80	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 395 and name CA)	17.53	0.40	0.39
	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 396 and name CA)	13.91	0.35	0.35
	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 396 and name CB)	13.09	0.43	0.43

	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 397 and name CA)	13.28	0.46	0.45
	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 397 and name CB)	13.83	0.57	0.57
	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 398 and name CA)	16.23	0.28	0.28
	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 398 and name CB)	17.62	0.30	0.30
5	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 399 and name CA)	15.35	0.37	0.37
	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 399 and name CB)	15.23	0.52	0.51
	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 400 and name CA)	12.05	0.29	0.29
	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 400 and name CB)	10.88	0.24	0.23
	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 401 and name CA)	14.01	0.24	0.24
	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 402 and name CA)	16.94	0.29	0.29
10	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 402 and name CB)	17.82	0.28	0.28
	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 403 and name CA)	15.39	0.60	0.60
	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 403 and name CB)	14.53	0.62	0.63
	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 404 and name CA)	13.61	0.72	0.72
	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 404 and name CB)	12.57	0.67	0.68
15	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 405 and name CA)	16.84	0.73	0.72
	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 405 and name CB)	17.46	0.62	0.62
	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 407 and name CA)	17.62	0.89	0.89
	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 407 and name CB)	16.44	0.92	0.92
	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 408 and name CA)	17.36	0.71	0.71
20	assign (segid 3A4 and resid 131 and name CB)	(segid 3A4 and resid 408 and name CB)	16.70	0.59	0.59
	assign (segid 3A4 and resid 131 and name N)	(segid 3A4 and resid 131 and name C)	2.46	0.03	0.03
	assign (segid 3A4 and resid 131 and name N)	(segid 3A4 and resid 131 and name CA)	1.45	0.01	0.01
	assign (segid 3A4 and resid 131 and name N)	(segid 3A4 and resid 131 and name CB)	2.46	0.04	0.05
25	assign (segid 3A4 and resid 131 and name N)	(segid 3A4 and resid 131 and name O)	3.50	0.03	0.03
	assign (segid 3A4 and resid 131 and name N)	(segid 3A4 and resid 132 and name C)	4.74	0.05	0.05
	assign (segid 3A4 and resid 131 and name N)	(segid 3A4 and resid 132 and name CA)	4.25	0.04	0.04
	assign (segid 3A4 and resid 131 and name N)	(segid 3A4 and resid 132 and name CB)	5.04	0.05	0.06
	assign (segid 3A4 and resid 131 and name N)	(segid 3A4 and resid 132 and name N)	2.85	0.04	0.05
30	assign (segid 3A4 and resid 131 and name N)	(segid 3A4 and resid 132 and name O)	5.84	0.06	0.06
	assign (segid 3A4 and resid 131 and name N)	(segid 3A4 and resid 133 and name C)	5.61	0.05	0.06
	assign (segid 3A4 and resid 131 and name N)	(segid 3A4 and resid 133 and name CA)	5.35	0.09	0.09
	assign (segid 3A4 and resid 131 and name N)	(segid 3A4 and resid 133 and name CB)	5.47	0.16	0.16
	assign (segid 3A4 and resid 131 and name N)	(segid 3A4 and resid 133 and name CG1)	6.00	0.19	0.19
35	assign (segid 3A4 and resid 131 and name N)	(segid 3A4 and resid 133 and name CG2)	6.72	0.16	0.16
	assign (segid 3A4 and resid 131 and name N)	(segid 3A4 and resid 133 and name N)	4.35	0.08	0.08
	assign (segid 3A4 and resid 131 and name N)	(segid 3A4 and resid 133 and name O)	6.81	0.06	0.05
	assign (segid 3A4 and resid 131 and name N)	(segid 3A4 and resid 134 and name C)	6.38	0.11	0.12
	assign (segid 3A4 and resid 131 and name N)	(segid 3A4 and resid 134 and name CA)	5.59	0.17	0.18
40	assign (segid 3A4 and resid 131 and name N)	(segid 3A4 and resid 134 and name N)	4.79	0.11	0.12
	assign (segid 3A4 and resid 131 and name N)	(segid 3A4 and resid 134 and name O)	7.60	0.13	0.13
	assign (segid 3A4 and resid 131 and name N)	(segid 3A4 and resid 135 and name CA)	7.10	0.06	0.07
	assign (segid 3A4 and resid 131 and name N)	(segid 3A4 and resid 135 and name CB)	6.87	0.09	0.09
	assign (segid 3A4 and resid 131 and name N)	(segid 3A4 and resid 135 and name N)	6.00	0.08	0.08
45	assign (segid 3A4 and resid 131 and name N)	(segid 3A4 and resid 256 and name CA)	6.29	0.81	0.82
	assign (segid 3A4 and resid 131 and name O)	(segid 3A4 and resid 131 and name CB)	3.29	0.05	0.06
	assign (segid 3A4 and resid 131 and name O)	(segid 3A4 and resid 132 and name C)	2.91	0.04	0.05
	assign (segid 3A4 and resid 131 and name O)	(segid 3A4 and resid 132 and name CA)	2.72	0.03	0.04
	assign (segid 3A4 and resid 131 and name O)	(segid 3A4 and resid 132 and name CB)	4.22	0.04	0.04
50	assign (segid 3A4 and resid 131 and name O)	(segid 3A4 and resid 132 and name N)	2.25	0.03	0.02
	assign (segid 3A4 and resid 131 and name O)	(segid 3A4 and resid 132 and name O)	3.41	0.11	0.11
	assign (segid 3A4 and resid 131 and name O)	(segid 3A4 and resid 133 and name C)	4.02	0.09	0.08
	assign (segid 3A4 and resid 131 and name O)	(segid 3A4 and resid 133 and name CA)	4.31	0.09	0.08
	assign (segid 3A4 and resid 131 and name O)	(segid 3A4 and resid 133 and name CB)	5.35	0.11	0.11
55	assign (segid 3A4 and resid 131 and name O)	(segid 3A4 and resid 133 and name CG1)	6.22	0.07	0.08
	assign (segid 3A4 and resid 131 and name O)	(segid 3A4 and resid 133 and name CG2)	6.45	0.12	0.13
	assign (segid 3A4 and resid 131 and name O)	(segid 3A4 and resid 133 and name N)	3.37	0.09	0.08
	assign (segid 3A4 and resid 131 and name O)	(segid 3A4 and resid 133 and name O)	4.90	0.07	0.07
	assign (segid 3A4 and resid 131 and name O)	(segid 3A4 and resid 134 and name C)	3.75	0.15	0.15
60	assign (segid 3A4 and resid 131 and name O)	(segid 3A4 and resid 134 and name CA)	3.78	0.18	0.18
	assign (segid 3A4 and resid 131 and name O)	(segid 3A4 and resid 134 and name N)	3.29	0.16	0.16
	assign (segid 3A4 and resid 131 and name O)	(segid 3A4 and resid 134 and name O)	4.92	0.14	0.15
	assign (segid 3A4 and resid 131 and name O)	(segid 3A4 and resid 135 and name C)	4.84	0.06	0.07
	assign (segid 3A4 and resid 131 and name O)	(segid 3A4 and resid 135 and name CA)	3.71	0.10	0.09
65	assign (segid 3A4 and resid 131 and name O)	(segid 3A4 and resid 135 and name CB)	3.39	0.09	0.08
	assign (segid 3A4 and resid 131 and name O)	(segid 3A4 and resid 135 and name N)	2.87	0.13	0.13
	assign (segid 3A4 and resid 131 and name O)	(segid 3A4 and resid 135 and name O)	5.98	0.08	0.07
	assign (segid 3A4 and resid 131 and name O)	(segid 3A4 and resid 136 and name C)	7.09	0.07	0.07
	assign (segid 3A4 and resid 131 and name O)	(segid 3A4 and resid 136 and name CA)	6.25	0.09	0.10
70	assign (segid 3A4 and resid 131 and name O)	(segid 3A4 and resid 136 and name CB)	6.53	0.17	0.17
	assign (segid 3A4 and resid 131 and name O)	(segid 3A4 and resid 136 and name N)	4.88	0.08	0.08
	assign (segid 3A4 and resid 131 and name O)	(segid 3A4 and resid 137 and name CA)	7.82	0.09	0.09
	assign (segid 3A4 and resid 131 and name O)	(segid 3A4 and resid 137 and name N)	6.72	0.07	0.07
	assign (segid 3A4 and resid 131 and name O)	(segid 3A4 and resid 138 and name N)	7.66	0.11	0.11
75	assign (segid 3A4 and resid 131 and name O)	(segid 3A4 and resid 140 and name CB)	7.42	0.34	0.35
	assign (segid 3A4 and resid 132 and name C)	(segid 3A4 and resid 132 and name CB)	2.49	0.01	0.01
	assign (segid 3A4 and resid 132 and name C)	(segid 3A4 and resid 132 and name O)	1.24	0.02	0.01
	assign (segid 3A4 and resid 132 and name C)	(segid 3A4 and resid 133 and name C)	3.03	0.02	0.03
	assign (segid 3A4 and resid 132 and name C)	(segid 3A4 and resid 133 and name CA)	2.43	0.02	0.01
80	assign (segid 3A4 and resid 132 and name C)	(segid 3A4 and resid 133 and name CB)	3.72	0.02	0.02
	assign (segid 3A4 and resid 132 and name C)	(segid 3A4 and resid 133 and name CG1)	4.13	0.05	0.05
	assign (segid 3A4 and resid 132 and name C)	(segid 3A4 and resid 133 and name CG2)	4.96	0.03	0.04
	assign (segid 3A4 and resid 132 and name C)	(segid 3A4 and resid 133 and name N)	1.33	0.01	0.00

	assign (segid 3A4 and resid 132 and name C)	(segid 3A4 and resid 133 and name O)	3.84	0.08	0.08
	assign (segid 3A4 and resid 132 and name C)	(segid 3A4 and resid 134 and name C)	4.57	0.10	0.10
	assign (segid 3A4 and resid 132 and name C)	(segid 3A4 and resid 134 and name CA)	4.54	0.11	0.10
	assign (segid 3A4 and resid 132 and name C)	(segid 3A4 and resid 134 and name N)	3.36	0.13	0.12
5	assign (segid 3A4 and resid 132 and name C)	(segid 3A4 and resid 134 and name O)	5.61	0.09	0.10
	assign (segid 3A4 and resid 132 and name C)	(segid 3A4 and resid 135 and name C)	4.83	0.07	0.07
	assign (segid 3A4 and resid 132 and name C)	(segid 3A4 and resid 135 and name CA)	4.53	0.11	0.10
	assign (segid 3A4 and resid 132 and name C)	(segid 3A4 and resid 135 and name CB)	4.37	0.16	0.16
	assign (segid 3A4 and resid 132 and name C)	(segid 3A4 and resid 135 and name N)	3.81	0.11	0.11
10	assign (segid 3A4 and resid 132 and name C)	(segid 3A4 and resid 135 and name O)	6.03	0.06	0.07
	assign (segid 3A4 and resid 132 and name C)	(segid 3A4 and resid 136 and name C)	6.03	0.16	0.17
	assign (segid 3A4 and resid 132 and name C)	(segid 3A4 and resid 136 and name CA)	5.01	0.11	0.12
	assign (segid 3A4 and resid 132 and name C)	(segid 3A4 and resid 136 and name CB)	4.64	0.21	0.21
	assign (segid 3A4 and resid 132 and name C)	(segid 3A4 and resid 136 and name N)	4.10	0.08	0.08
15	assign (segid 3A4 and resid 132 and name C)	(segid 3A4 and resid 136 and name O)	7.17	0.17	0.17
	assign (segid 3A4 and resid 132 and name C)	(segid 3A4 and resid 137 and name CA)	7.12	0.26	0.26
	assign (segid 3A4 and resid 132 and name C)	(segid 3A4 and resid 137 and name N)	5.88	0.21	0.20
	assign (segid 3A4 and resid 132 and name C)	(segid 3A4 and resid 138 and name N)	7.78	0.09	0.10
	assign (segid 3A4 and resid 132 and name C)	(segid 3A4 and resid 140 and name O)	7.21	0.27	0.27
20	assign (segid 3A4 and resid 132 and name C)	(segid 3A4 and resid 132 and name C)	1.52	0.01	0.01
	assign (segid 3A4 and resid 132 and name CA)	(segid 3A4 and resid 132 and name CB)	1.53	0.02	0.01
	assign (segid 3A4 and resid 132 and name CA)	(segid 3A4 and resid 132 and name O)	2.40	0.02	0.01
	assign (segid 3A4 and resid 132 and name CA)	(segid 3A4 and resid 133 and name C)	4.41	0.02	0.02
	assign (segid 3A4 and resid 132 and name CA)	(segid 3A4 and resid 133 and name CA)	3.80	0.01	0.00
25	assign (segid 3A4 and resid 132 and name CA)	(segid 3A4 and resid 133 and name CB)	4.88	0.04	0.03
	assign (segid 3A4 and resid 132 and name CA)	(segid 3A4 and resid 133 and name CG1)	5.08	0.05	0.06
	assign (segid 3A4 and resid 132 and name CA)	(segid 3A4 and resid 133 and name CG2)	6.26	0.03	0.02
	assign (segid 3A4 and resid 132 and name CA)	(segid 3A4 and resid 133 and name N)	2.43	0.02	0.02
	assign (segid 3A4 and resid 132 and name CA)	(segid 3A4 and resid 133 and name O)	5.29	0.08	0.08
30	assign (segid 3A4 and resid 132 and name CA)	(segid 3A4 and resid 134 and name C)	5.50	0.11	0.11
	assign (segid 3A4 and resid 132 and name CA)	(segid 3A4 and resid 134 and name CA)	5.51	0.12	0.13
	assign (segid 3A4 and resid 132 and name CA)	(segid 3A4 and resid 134 and name N)	4.43	0.13	0.13
	assign (segid 3A4 and resid 132 and name CA)	(segid 3A4 and resid 134 and name O)	6.60	0.09	0.10
	assign (segid 3A4 and resid 132 and name CA)	(segid 3A4 and resid 135 and name C)	5.64	0.05	0.05
35	assign (segid 3A4 and resid 132 and name CA)	(segid 3A4 and resid 135 and name CA)	5.09	0.10	0.10
	assign (segid 3A4 and resid 132 and name CA)	(segid 3A4 and resid 135 and name CB)	4.50	0.14	0.13
	assign (segid 3A4 and resid 132 and name CA)	(segid 3A4 and resid 135 and name N)	4.54	0.11	0.11
	assign (segid 3A4 and resid 132 and name CA)	(segid 3A4 and resid 135 and name O)	6.82	0.05	0.05
	assign (segid 3A4 and resid 132 and name CA)	(segid 3A4 and resid 136 and name C)	7.28	0.16	0.16
40	assign (segid 3A4 and resid 132 and name CA)	(segid 3A4 and resid 136 and name CA)	6.13	0.15	0.16
	assign (segid 3A4 and resid 132 and name CA)	(segid 3A4 and resid 136 and name CB)	5.83	0.24	0.24
	assign (segid 3A4 and resid 132 and name CA)	(segid 3A4 and resid 136 and name N)	5.12	0.10	0.10
	assign (segid 3A4 and resid 132 and name CA)	(segid 3A4 and resid 137 and name CA)	8.50	0.23	0.23
	assign (segid 3A4 and resid 132 and name CA)	(segid 3A4 and resid 137 and name N)	7.22	0.19	0.19
45	assign (segid 3A4 and resid 132 and name CA)	(segid 3A4 and resid 138 and name CA)	9.94	0.07	0.07
	assign (segid 3A4 and resid 132 and name CA)	(segid 3A4 and resid 138 and name CB)	9.81	0.40	0.40
	assign (segid 3A4 and resid 132 and name CA)	(segid 3A4 and resid 139 and name CA)	9.95	0.39	0.39
	assign (segid 3A4 and resid 132 and name CA)	(segid 3A4 and resid 140 and name CA)	9.14	0.19	0.20
	assign (segid 3A4 and resid 132 and name CA)	(segid 3A4 and resid 140 and name CB)	9.02	0.73	0.74
50	assign (segid 3A4 and resid 132 and name CA)	(segid 3A4 and resid 140 and name O)	7.43	0.25	0.26
	assign (segid 3A4 and resid 132 and name CA)	(segid 3A4 and resid 141 and name CA)	9.01	0.67	0.67
	assign (segid 3A4 and resid 132 and name CA)	(segid 3A4 and resid 141 and name CB)	9.98	1.22	1.23
	assign (segid 3A4 and resid 132 and name CA)	(segid 3A4 and resid 147 and name CA)	11.04	3.59	3.58
	assign (segid 3A4 and resid 132 and name CA)	(segid 3A4 and resid 147 and name CB)	11.69	4.00	3.99
55	assign (segid 3A4 and resid 132 and name CA)	(segid 3A4 and resid 148 and name CA)	12.44	1.84	1.84
	assign (segid 3A4 and resid 132 and name CA)	(segid 3A4 and resid 149 and name CA)	11.24	1.01	1.01
	assign (segid 3A4 and resid 132 and name CA)	(segid 3A4 and resid 149 and name CB)	11.13	0.57	0.57
	assign (segid 3A4 and resid 132 and name CA)	(segid 3A4 and resid 150 and name CA)	10.26	3.15	3.15
	assign (segid 3A4 and resid 132 and name CA)	(segid 3A4 and resid 151 and name CA)	12.52	2.94	2.94
60	assign (segid 3A4 and resid 132 and name CA)	(segid 3A4 and resid 152 and name CA)	13.18	1.30	1.30
	assign (segid 3A4 and resid 132 and name CA)	(segid 3A4 and resid 152 and name CB)	13.17	0.84	0.83
	assign (segid 3A4 and resid 132 and name CA)	(segid 3A4 and resid 153 and name CA)	12.07	1.98	1.98
	assign (segid 3A4 and resid 132 and name CA)	(segid 3A4 and resid 153 and name CB)	11.34	2.17	2.17
	assign (segid 3A4 and resid 132 and name CA)	(segid 3A4 and resid 155 and name CB)	15.81	2.02	2.02
65	assign (segid 3A4 and resid 132 and name CA)	(segid 3A4 and resid 156 and name CA)	15.51	1.82	1.81
	assign (segid 3A4 and resid 132 and name CA)	(segid 3A4 and resid 156 and name CB)	14.86	1.70	1.70
	assign (segid 3A4 and resid 132 and name CA)	(segid 3A4 and resid 194 and name CA)	16.83	1.04	1.04
	assign (segid 3A4 and resid 132 and name CA)	(segid 3A4 and resid 194 and name CB)	16.43	1.11	1.11
	assign (segid 3A4 and resid 132 and name CA)	(segid 3A4 and resid 197 and name CA)	16.82	0.71	0.71
70	assign (segid 3A4 and resid 132 and name CA)	(segid 3A4 and resid 197 and name CB)	15.74	0.75	0.74
	assign (segid 3A4 and resid 132 and name CA)	(segid 3A4 and resid 198 and name CA)	16.10	0.78	0.78
	assign (segid 3A4 and resid 132 and name CA)	(segid 3A4 and resid 198 and name CB)	16.04	0.80	0.79
	assign (segid 3A4 and resid 132 and name CA)	(segid 3A4 and resid 201 and name CA)	16.58	0.73	0.74
	assign (segid 3A4 and resid 132 and name CA)	(segid 3A4 and resid 201 and name CB)	15.19	0.71	0.70
75	assign (segid 3A4 and resid 132 and name CA)	(segid 3A4 and resid 202 and name CA)	18.62	0.73	0.74
	assign (segid 3A4 and resid 132 and name CA)	(segid 3A4 and resid 205 and name CB)	17.92	0.70	0.71
	assign (segid 3A4 and resid 132 and name CA)	(segid 3A4 and resid 219 and name CA)	12.78	0.94	0.95
	assign (segid 3A4 and resid 132 and name CA)	(segid 3A4 and resid 219 and name CB)	12.09	0.88	0.87
	assign (segid 3A4 and resid 132 and name CA)	(segid 3A4 and resid 220 and name CA)	13.47	0.81	0.80
80	assign (segid 3A4 and resid 132 and name CA)	(segid 3A4 and resid 220 and name CB)	12.66	0.79	0.79
	assign (segid 3A4 and resid 132 and name CA)	(segid 3A4 and resid 221 and name CA)	14.93	0.48	0.49
	assign (segid 3A4 and resid 132 and name CA)	(segid 3A4 and resid 221 and name CB)	14.41	0.36	0.36
	assign (segid 3A4 and resid 132 and name CA)	(segid 3A4 and resid 222 and name CA)	17.29	0.62	0.62

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	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 136 and name CA)	6.91	0.17	0.17
	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 136 and name CB)	6.33	0.27	0.26
	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 136 and name N)	6.13	0.11	0.10
	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 137 and name CA)	9.49	0.27	0.28
	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 138 and name CA)	11.21	0.09	0.09
5	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 138 and name CB)	11.16	0.37	0.38
	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 139 and name CA)	11.04	0.26	0.27
	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 140 and name CA)	10.30	0.34	0.35
	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 140 and name CB)	10.27	0.89	0.88
	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 141 and name CA)	9.83	0.38	0.38
10	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 141 and name CB)	10.74	0.93	0.94
	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 147 and name CA)	11.44	3.97	3.97
	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 147 and name CB)	11.94	4.50	4.50
	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 148 and name CA)	12.89	2.27	2.26
	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 149 and name CA)	11.94	1.21	1.21
15	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 149 and name CB)	11.92	0.71	0.72
	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 150 and name CA)	10.88	3.27	3.27
	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 151 and name CA)	13.02	3.18	3.17
	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 152 and name CA)	13.87	1.40	1.40
	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 152 and name CB)	13.89	0.90	0.91
20	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 153 and name CA)	12.89	1.86	1.86
	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 153 and name CB)	12.20	2.01	2.01
	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 156 and name CA)	16.27	1.73	1.73
	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 156 and name CB)	15.66	1.67	1.66
	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 194 and name CA)	18.00	1.06	1.05
25	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 194 and name CB)	17.58	1.11	1.11
	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 197 and name CA)	18.03	0.72	0.71
	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 197 and name CB)	16.93	0.76	0.76
	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 198 and name CA)	17.38	0.81	0.81
	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 198 and name CB)	17.32	0.86	0.87
30	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 201 and name CA)	17.81	0.68	0.67
	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 201 and name CB)	16.43	0.65	0.64
	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 219 and name CA)	13.66	1.01	1.01
	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 219 and name CB)	13.02	0.88	0.89
	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 220 and name CA)	14.45	1.02	1.02
35	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 220 and name CB)	13.67	1.04	1.04
	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 221 and name CA)	16.07	0.61	0.62
	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 221 and name CB)	15.60	0.44	0.43
	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 222 and name CA)	18.31	0.70	0.70
	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 222 and name CB)	18.07	0.66	0.67
40	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 223 and name CB)	18.55	1.11	1.11
	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 248 and name CA)	15.64	1.43	1.42
	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 248 and name CB)	15.78	1.34	1.33
	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 249 and name CA)	16.10	1.15	1.15
	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 250 and name CA)	16.53	1.22	1.21
45	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 250 and name CB)	17.65	1.29	1.30
	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 251 and name CA)	13.46	1.44	1.45
	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 251 and name CB)	13.25	1.63	1.63
	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 252 and name CA)	11.45	1.00	1.01
	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 252 and name CB)	11.82	0.96	0.96
50	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 253 and name CA)	13.67	0.67	0.68
	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 254 and name CA)	14.30	1.03	1.04
	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 255 and name CA)	11.12	1.49	1.48
	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 256 and name CA)	9.73	0.87	0.87
	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 257 and name CA)	12.70	0.66	0.66
55	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 258 and name CA)	13.97	0.99	0.98
	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 258 and name CB)	14.42	1.18	1.19
	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 259 and name CA)	11.37	1.13	1.14
	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 259 and name CB)	10.14	1.26	1.26
	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 260 and name CA)	11.16	0.62	0.63
60	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 260 and name CB)	11.02	0.60	0.60
	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 261 and name CA)	14.91	0.66	0.67
	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 262 and name CA)	15.37	0.98	0.98
	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 262 and name CB)	14.98	1.15	1.16
	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 263 and name CA)	13.75	0.75	0.75
65	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 263 and name CB)	12.34	0.70	0.69
	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 264 and name CA)	15.87	0.49	0.49
	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 265 and name CA)	18.83	0.74	0.73
	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 266 and name CA)	18.57	0.82	0.83
	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 267 and name CA)	18.76	0.45	0.45
70	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 267 and name CB)	17.78	0.40	0.39
	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 293 and name CA)	14.61	1.96	1.96
	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 394 and name CA)	16.39	1.92	1.93
	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 394 and name CB)	17.89	1.93	1.94
	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 395 and name CA)	15.76	1.98	1.97
75	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 396 and name CA)	12.00	1.95	1.95
	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 396 and name CB)	11.33	1.97	1.98
	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 397 and name CA)	12.16	1.97	1.96
	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 397 and name CB)	13.10	1.96	1.97
	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 398 and name CA)	14.63	1.87	1.88
80	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 398 and name CB)	15.99	1.91	1.91
	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 399 and name CA)	12.94	1.77	1.76
	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 399 and name CB)	12.61	1.82	1.82

	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 400 and name CA)	9.88	1.67	1.67
	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 400 and name CB)	8.94	1.69	1.68
	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 401 and name CA)	12.59	1.60	1.60
	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 402 and name CA)	14.88	1.50	1.51
	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 402 and name CB)	15.61	1.54	1.53
5	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 403 and name CA)	17.79	1.23	1.24
	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 403 and name CB)	11.71	1.20	1.20
	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 404 and name CA)	11.78	1.26	1.25
	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 404 and name CB)	11.08	1.39	1.39
	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 405 and name CA)	15.33	1.39	1.39
	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 405 and name CB)	16.07	1.50	1.50
10	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 406 and name CA)	16.92	1.17	1.16
	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 407 and name CA)	15.37	0.76	0.76
	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 407 and name CB)	14.06	0.70	0.71
	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 408 and name CA)	15.89	0.51	0.52
	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 408 and name CB)	15.52	0.58	0.58
15	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 411 and name CB)	18.17	0.40	0.40
	assign (segid 3A4 and resid 132 and name CB)	(segid 3A4 and resid 132 and name C)	2.46	0.02	0.02
	assign (segid 3A4 and resid 132 and name N)	(segid 3A4 and resid 132 and name CA)	1.46	0.00	0.01
	assign (segid 3A4 and resid 132 and name N)	(segid 3A4 and resid 132 and name CB)	2.46	0.03	0.02
20	assign (segid 3A4 and resid 132 and name N)	(segid 3A4 and resid 132 and name O)	3.52	0.04	0.04
	assign (segid 3A4 and resid 132 and name N)	(segid 3A4 and resid 133 and name C)	4.70	0.06	0.05
	assign (segid 3A4 and resid 132 and name N)	(segid 3A4 and resid 133 and name CA)	4.21	0.04	0.04
	assign (segid 3A4 and resid 132 and name N)	(segid 3A4 and resid 133 and name CB)	5.00	0.07	0.07
	assign (segid 3A4 and resid 132 and name N)	(segid 3A4 and resid 133 and name CG1)	5.33	0.09	0.10
25	assign (segid 3A4 and resid 132 and name N)	(segid 3A4 and resid 133 and name CG2)	6.42	0.05	0.06
	assign (segid 3A4 and resid 132 and name N)	(segid 3A4 and resid 133 and name N)	2.81	0.04	0.04
	assign (segid 3A4 and resid 132 and name N)	(segid 3A4 and resid 133 and name O)	5.76	0.07	0.06
	assign (segid 3A4 and resid 132 and name N)	(segid 3A4 and resid 134 and name C)	5.61	0.12	0.12
	assign (segid 3A4 and resid 132 and name N)	(segid 3A4 and resid 134 and name CA)	5.38	0.17	0.16
30	assign (segid 3A4 and resid 132 and name N)	(segid 3A4 and resid 134 and name N)	4.35	0.14	0.15
	assign (segid 3A4 and resid 132 and name N)	(segid 3A4 and resid 134 and name O)	6.81	0.11	0.11
	assign (segid 3A4 and resid 132 and name N)	(segid 3A4 and resid 135 and name C)	6.38	0.06	0.05
	assign (segid 3A4 and resid 132 and name N)	(segid 3A4 and resid 135 and name CA)	5.54	0.10	0.09
35	assign (segid 3A4 and resid 132 and name N)	(segid 3A4 and resid 135 and name CB)	4.99	0.11	0.12
	assign (segid 3A4 and resid 132 and name N)	(segid 3A4 and resid 135 and name N)	4.77	0.10	0.10
	assign (segid 3A4 and resid 132 and name N)	(segid 3A4 and resid 135 and name O)	7.57	0.05	0.05
	assign (segid 3A4 and resid 132 and name N)	(segid 3A4 and resid 136 and name CA)	7.19	0.13	0.13
	assign (segid 3A4 and resid 132 and name N)	(segid 3A4 and resid 136 and name CB)	7.01	0.21	0.21
40	assign (segid 3A4 and resid 132 and name N)	(segid 3A4 and resid 136 and name N)	6.04	0.09	0.09
	assign (segid 3A4 and resid 132 and name O)	(segid 3A4 and resid 132 and name CB)	3.27	0.06	0.05
	assign (segid 3A4 and resid 132 and name O)	(segid 3A4 and resid 133 and name C)	3.01	0.06	0.05
	assign (segid 3A4 and resid 132 and name O)	(segid 3A4 and resid 133 and name CA)	2.75	0.03	0.02
	assign (segid 3A4 and resid 132 and name O)	(segid 3A4 and resid 133 and name CB)	4.25	0.04	0.03
	assign (segid 3A4 and resid 132 and name O)	(segid 3A4 and resid 133 and name CG1)	4.74	0.07	0.07
45	assign (segid 3A4 and resid 132 and name O)	(segid 3A4 and resid 133 and name CG2)	5.23	0.06	0.06
	assign (segid 3A4 and resid 132 and name O)	(segid 3A4 and resid 133 and name N)	2.24	0.01	0.02
	assign (segid 3A4 and resid 132 and name O)	(segid 3A4 and resid 133 and name O)	3.44	0.13	0.13
	assign (segid 3A4 and resid 132 and name O)	(segid 3A4 and resid 134 and name C)	4.20	0.13	0.14
	assign (segid 3A4 and resid 132 and name O)	(segid 3A4 and resid 134 and name CA)	4.52	0.13	0.13
50	assign (segid 3A4 and resid 132 and name O)	(segid 3A4 and resid 134 and name N)	3.56	0.14	0.14
	assign (segid 3A4 and resid 132 and name O)	(segid 3A4 and resid 134 and name O)	5.07	0.12	0.12
	assign (segid 3A4 and resid 132 and name O)	(segid 3A4 and resid 135 and name C)	3.84	0.12	0.11
	assign (segid 3A4 and resid 132 and name O)	(segid 3A4 and resid 135 and name CA)	3.84	0.17	0.17
	assign (segid 3A4 and resid 132 and name O)	(segid 3A4 and resid 135 and name CB)	3.80	0.22	0.21
55	assign (segid 3A4 and resid 132 and name O)	(segid 3A4 and resid 135 and name N)	3.40	0.18	0.17
	assign (segid 3A4 and resid 132 and name O)	(segid 3A4 and resid 135 and name O)	5.00	0.11	0.11
	assign (segid 3A4 and resid 132 and name O)	(segid 3A4 and resid 136 and name C)	4.95	0.18	0.17
	assign (segid 3A4 and resid 132 and name O)	(segid 3A4 and resid 136 and name CA)	3.83	0.13	0.13
60	assign (segid 3A4 and resid 132 and name O)	(segid 3A4 and resid 136 and name CB)	3.52	0.24	0.24
	assign (segid 3A4 and resid 132 and name O)	(segid 3A4 and resid 136 and name N)	2.99	0.10	0.10
	assign (segid 3A4 and resid 132 and name O)	(segid 3A4 and resid 136 and name O)	6.06	0.18	0.17
	assign (segid 3A4 and resid 132 and name O)	(segid 3A4 and resid 137 and name C)	7.22	0.21	0.20
	assign (segid 3A4 and resid 132 and name O)	(segid 3A4 and resid 137 and name CA)	6.29	0.27	0.28
	assign (segid 3A4 and resid 132 and name O)	(segid 3A4 and resid 137 and name N)	4.96	0.23	0.23
65	assign (segid 3A4 and resid 132 and name O)	(segid 3A4 and resid 138 and name N)	6.96	0.10	0.10
	assign (segid 3A4 and resid 132 and name O)	(segid 3A4 and resid 139 and name N)	7.58	0.18	0.19
	assign (segid 3A4 and resid 132 and name O)	(segid 3A4 and resid 140 and name C)	7.56	0.19	0.20
	assign (segid 3A4 and resid 132 and name O)	(segid 3A4 and resid 140 and name N)	7.64	0.11	0.12
	assign (segid 3A4 and resid 132 and name O)	(segid 3A4 and resid 140 and name O)	6.47	0.18	0.18
70	assign (segid 3A4 and resid 133 and name O)	(segid 3A4 and resid 133 and name CB)	2.54	0.03	0.02
	assign (segid 3A4 and resid 133 and name C)	(segid 3A4 and resid 133 and name CG1)	3.86	0.02	0.02
	assign (segid 3A4 and resid 133 and name C)	(segid 3A4 and resid 133 and name CG2)	2.93	0.05	0.05
	assign (segid 3A4 and resid 133 and name C)	(segid 3A4 and resid 133 and name O)	1.24	0.01	0.00
	assign (segid 3A4 and resid 133 and name C)	(segid 3A4 and resid 134 and name C)	3.00	0.05	0.04
75	assign (segid 3A4 and resid 133 and name C)	(segid 3A4 and resid 134 and name CA)	2.42	0.00	0.01
	assign (segid 3A4 and resid 133 and name C)	(segid 3A4 and resid 134 and name N)	1.33	0.01	0.01
	assign (segid 3A4 and resid 133 and name C)	(segid 3A4 and resid 134 and name O)	3.83	0.08	0.08
	assign (segid 3A4 and resid 133 and name C)	(segid 3A4 and resid 135 and name C)	4.54	0.04	0.04
	assign (segid 3A4 and resid 133 and name C)	(segid 3A4 and resid 135 and name CA)	4.45	0.05	0.04
80	assign (segid 3A4 and resid 133 and name C)	(segid 3A4 and resid 135 and name CB)	5.24	0.08	0.07
	assign (segid 3A4 and resid 133 and name C)	(segid 3A4 and resid 135 and name N)	3.25	0.03	0.03
	assign (segid 3A4 and resid 133 and name C)	(segid 3A4 and resid 135 and name O)	5.58	0.07	0.08

5	assign (segid 3A4 and resid 133 and name C) (segid 3A4 and resid 136 and name C)	4.83	0.07	0.07
	assign (segid 3A4 and resid 133 and name C) (segid 3A4 and resid 136 and name CA)	4.59	0.10	0.11
	assign (segid 3A4 and resid 133 and name C) (segid 3A4 and resid 136 and name CB)	4.48	0.30	0.30
	assign (segid 3A4 and resid 133 and name C) (segid 3A4 and resid 136 and name N)	3.84	0.08	0.09
	assign (segid 3A4 and resid 133 and name C) (segid 3A4 and resid 136 and name O)	6.00	0.09	0.08
10	assign (segid 3A4 and resid 133 and name C) (segid 3A4 and resid 137 and name C)	5.97	0.23	0.22
	assign (segid 3A4 and resid 133 and name C) (segid 3A4 and resid 137 and name CA)	4.91	0.23	0.22
	assign (segid 3A4 and resid 133 and name C) (segid 3A4 and resid 137 and name N)	4.07	0.12	0.12
	assign (segid 3A4 and resid 133 and name C) (segid 3A4 and resid 137 and name O)	7.11	0.23	0.24
	assign (segid 3A4 and resid 133 and name C) (segid 3A4 and resid 138 and name CA)	7.09	0.19	0.20
15	assign (segid 3A4 and resid 133 and name C) (segid 3A4 and resid 138 and name CB)	7.14	0.15	0.16
	assign (segid 3A4 and resid 133 and name C) (segid 3A4 and resid 138 and name N)	5.84	0.21	0.20
	assign (segid 3A4 and resid 133 and name C) (segid 3A4 and resid 139 and name N)	7.45	0.38	0.37
	assign (segid 3A4 and resid 133 and name CA) (segid 3A4 and resid 133 and name C)	1.53	0.01	0.00
	assign (segid 3A4 and resid 133 and name CA) (segid 3A4 and resid 133 and name CB)	1.55	0.01	0.01
20	assign (segid 3A4 and resid 133 and name CA) (segid 3A4 and resid 133 and name CG1)	2.50	0.01	0.02
	assign (segid 3A4 and resid 133 and name CA) (segid 3A4 and resid 133 and name CG2)	2.56	0.03	0.03
	assign (segid 3A4 and resid 133 and name CA) (segid 3A4 and resid 133 and name O)	2.39	0.02	0.01
	assign (segid 3A4 and resid 133 and name CA) (segid 3A4 and resid 131 and name C)	4.39	0.06	0.06
	assign (segid 3A4 and resid 133 and name CA) (segid 3A4 and resid 134 and name CA)	3.81	0.01	0.01
25	assign (segid 3A4 and resid 133 and name CA) (segid 3A4 and resid 134 and name N)	2.44	0.03	0.03
	assign (segid 3A4 and resid 133 and name CA) (segid 3A4 and resid 134 and name O)	5.29	0.10	0.09
	assign (segid 3A4 and resid 133 and name CA) (segid 3A4 and resid 135 and name C)	5.46	0.10	0.11
	assign (segid 3A4 and resid 133 and name CA) (segid 3A4 and resid 135 and name CA)	5.42	0.09	0.09
	assign (segid 3A4 and resid 133 and name CA) (segid 3A4 and resid 135 and name CB)	5.89	0.13	0.12
30	assign (segid 3A4 and resid 133 and name CA) (segid 3A4 and resid 135 and name N)	4.33	0.06	0.07
	assign (segid 3A4 and resid 133 and name CA) (segid 3A4 and resid 135 and name O)	6.58	0.13	0.12
	assign (segid 3A4 and resid 133 and name CA) (segid 3A4 and resid 136 and name C)	5.64	0.18	0.18
	assign (segid 3A4 and resid 133 and name CA) (segid 3A4 and resid 136 and name CA)	5.16	0.09	0.09
	assign (segid 3A4 and resid 133 and name CA) (segid 3A4 and resid 136 and name CB)	4.62	0.21	0.21
35	assign (segid 3A4 and resid 133 and name CA) (segid 3A4 and resid 136 and name N)	4.56	0.10	0.09
	assign (segid 3A4 and resid 133 and name CA) (segid 3A4 and resid 136 and name O)	6.75	0.22	0.23
	assign (segid 3A4 and resid 133 and name CA) (segid 3A4 and resid 137 and name C)	7.22	0.31	0.31
	assign (segid 3A4 and resid 133 and name CA) (segid 3A4 and resid 137 and name CA)	6.02	0.33	0.33
	assign (segid 3A4 and resid 133 and name CA) (segid 3A4 and resid 137 and name N)	5.10	0.22	0.23
40	assign (segid 3A4 and resid 133 and name CA) (segid 3A4 and resid 138 and name CA)	8.49	0.21	0.22
	assign (segid 3A4 and resid 133 and name CA) (segid 3A4 and resid 138 and name CB)	8.58	0.15	0.15
	assign (segid 3A4 and resid 133 and name CA) (segid 3A4 and resid 138 and name N)	7.20	0.25	0.24
	assign (segid 3A4 and resid 133 and name CA) (segid 3A4 and resid 139 and name CA)	9.54	0.41	0.41
	assign (segid 3A4 and resid 133 and name CA) (segid 3A4 and resid 140 and name CA)	9.79	0.33	0.32
45	assign (segid 3A4 and resid 133 and name CA) (segid 3A4 and resid 140 and name CB)	9.65	0.42	0.42
	assign (segid 3A4 and resid 133 and name CA) (segid 3A4 and resid 141 and name CA)	10.61	0.88	0.87
	assign (segid 3A4 and resid 133 and name CA) (segid 3A4 and resid 141 and name CB)	11.80	1.25	1.25
	assign (segid 3A4 and resid 133 and name CA) (segid 3A4 and resid 147 and name CA)	12.74	2.46	2.47
	assign (segid 3A4 and resid 133 and name CA) (segid 3A4 and resid 147 and name CB)	13.36	2.87	2.88
50	assign (segid 3A4 and resid 133 and name CA) (segid 3A4 and resid 148 and name CA)	14.13	0.72	0.72
	assign (segid 3A4 and resid 133 and name CA) (segid 3A4 and resid 149 and name CA)	12.93	0.58	0.58
	assign (segid 3A4 and resid 133 and name CA) (segid 3A4 and resid 149 and name CB)	12.75	0.64	0.64
	assign (segid 3A4 and resid 133 and name CA) (segid 3A4 and resid 150 and name CA)	12.24	1.73	1.73
	assign (segid 3A4 and resid 133 and name CA) (segid 3A4 and resid 151 and name CA)	14.37	1.31	1.30
55	assign (segid 3A4 and resid 133 and name CA) (segid 3A4 and resid 152 and name CA)	14.61	1.24	1.23
	assign (segid 3A4 and resid 133 and name CA) (segid 3A4 and resid 152 and name CB)	14.55	1.84	1.85
	assign (segid 3A4 and resid 133 and name CA) (segid 3A4 and resid 153 and name CA)	13.29	1.06	1.07
	assign (segid 3A4 and resid 133 and name CA) (segid 3A4 and resid 153 and name CB)	12.59	1.19	1.19
	assign (segid 3A4 and resid 133 and name CA) (segid 3A4 and resid 154 and name CA)	14.21	2.00	2.00
60	assign (segid 3A4 and resid 133 and name CA) (segid 3A4 and resid 155 and name CA)	16.56	1.	

	assign (segid 3A4 and resid 133 and name CA)	(segid 3A4 and resid 224 and name CB)	16.15	1.12	1.12
	assign (segid 3A4 and resid 133 and name CA)	(segid 3A4 and resid 225 and name CB)	18.83	1.01	1.00
	assign (segid 3A4 and resid 133 and name CA)	(segid 3A4 and resid 247 and name CA)	15.46	2.11	2.10
	assign (segid 3A4 and resid 133 and name CA)	(segid 3A4 and resid 247 and name CB)	15.71	2.08	2.07
5	assign (segid 3A4 and resid 133 and name CA)	(segid 3A4 and resid 248 and name CA)	12.62	2.17	2.18
	assign (segid 3A4 and resid 133 and name CA)	(segid 3A4 and resid 248 and name CB)	12.91	2.16	2.16
	assign (segid 3A4 and resid 133 and name CA)	(segid 3A4 and resid 249 and name CA)	13.58	2.00	2.00
	assign (segid 3A4 and resid 133 and name CA)	(segid 3A4 and resid 250 and name CA)	13.71	1.75	1.75
	assign (segid 3A4 and resid 133 and name CA)	(segid 3A4 and resid 250 and name CB)	14.69	1.74	1.74
10	assign (segid 3A4 and resid 133 and name CA)	(segid 3A4 and resid 251 and name CA)	10.33	1.76	1.76
	assign (segid 3A4 and resid 133 and name CA)	(segid 3A4 and resid 251 and name CB)	9.92	1.95	1.95
	assign (segid 3A4 and resid 133 and name CA)	(segid 3A4 and resid 252 and name CA)	9.04	1.61	1.62
	assign (segid 3A4 and resid 133 and name CA)	(segid 3A4 and resid 252 and name CB)	9.63	1.72	1.72
	assign (segid 3A4 and resid 133 and name CA)	(segid 3A4 and resid 253 and name CA)	11.77	1.18	1.17
	assign (segid 3A4 and resid 133 and name CA)	(segid 3A4 and resid 254 and name CA)	11.99	1.02	1.02
15	assign (segid 3A4 and resid 133 and name CA)	(segid 3A4 and resid 255 and name CA)	8.90	1.29	1.28
	assign (segid 3A4 and resid 133 and name CA)	(segid 3A4 and resid 256 and name CA)	8.64	0.85	0.86
	assign (segid 3A4 and resid 133 and name CA)	(segid 3A4 and resid 257 and name CA)	12.12	0.63	0.62
	assign (segid 3A4 and resid 133 and name CA)	(segid 3A4 and resid 258 and name CA)	12.96	0.45	0.45
	assign (segid 3A4 and resid 133 and name CA)	(segid 3A4 and resid 258 and name CB)	13.05	0.60	0.59
20	assign (segid 3A4 and resid 133 and name CA)	(segid 3A4 and resid 259 and name CA)	10.72	0.27	0.27
	assign (segid 3A4 and resid 133 and name CA)	(segid 3A4 and resid 259 and name CB)	9.31	0.30	0.30
	assign (segid 3A4 and resid 133 and name CA)	(segid 3A4 and resid 260 and name CA)	11.62	0.24	0.25
	assign (segid 3A4 and resid 133 and name CA)	(segid 3A4 and resid 260 and name CB)	11.61	0.30	0.30
	assign (segid 3A4 and resid 133 and name CA)	(segid 3A4 and resid 261 and name CA)	15.13	0.24	0.25
25	assign (segid 3A4 and resid 133 and name CA)	(segid 3A4 and resid 262 and name CA)	15.31	0.33	0.33
	assign (segid 3A4 and resid 133 and name CA)	(segid 3A4 and resid 262 and name CB)	14.63	0.38	0.39
	assign (segid 3A4 and resid 133 and name CA)	(segid 3A4 and resid 263 and name CA)	14.43	0.54	0.54
	assign (segid 3A4 and resid 133 and name CA)	(segid 3A4 and resid 263 and name CB)	13.19	0.58	0.58
	assign (segid 3A4 and resid 133 and name CA)	(segid 3A4 and resid 264 and name CA)	16.97	0.42	0.42
30	assign (segid 3A4 and resid 133 and name CA)	(segid 3A4 and resid 265 and name CA)	19.45	0.38	0.37
	assign (segid 3A4 and resid 133 and name CA)	(segid 3A4 and resid 309 and name CB)	17.73	1.05	1.04
	assign (segid 3A4 and resid 133 and name CA)	(segid 3A4 and resid 313 and name CB)	18.99	0.74	0.75
	assign (segid 3A4 and resid 133 and name CA)	(segid 3A4 and resid 318 and name CB)	17.81	0.93	0.93
	assign (segid 3A4 and resid 133 and name CA)	(segid 3A4 and resid 384 and name CA)	18.61	0.64	0.64
35	assign (segid 3A4 and resid 133 and name CA)	(segid 3A4 and resid 384 and name CB)	18.01	0.67	0.68
	assign (segid 3A4 and resid 133 and name CA)	(segid 3A4 and resid 391 and name CA)	16.42	1.00	0.99
	assign (segid 3A4 and resid 133 and name CA)	(segid 3A4 and resid 391 and name CB)	15.83	0.93	0.93
	assign (segid 3A4 and resid 133 and name CA)	(segid 3A4 and resid 392 and name CA)	14.79	1.04	1.05
40	assign (segid 3A4 and resid 133 and name CA)	(segid 3A4 and resid 392 and name CB)	14.66	1.14	1.15
	assign (segid 3A4 and resid 133 and name CA)	(segid 3A4 and resid 393 and name CA)	11.57	0.85	0.85
	assign (segid 3A4 and resid 133 and name CA)	(segid 3A4 and resid 394 and name CA)	13.83	0.52	0.51
	assign (segid 3A4 and resid 133 and name CA)	(segid 3A4 and resid 394 and name CB)	15.31	0.54	0.54
	assign (segid 3A4 and resid 133 and name CA)	(segid 3A4 and resid 395 and name CA)	13.23	0.32	0.33
	assign (segid 3A4 and resid 133 and name CA)	(segid 3A4 and resid 396 and name CA)	9.56	0.26	0.25
45	assign (segid 3A4 and resid 133 and name CA)	(segid 3A4 and resid 396 and name CB)	8.62	0.29	0.30
	assign (segid 3A4 and resid 133 and name CA)	(segid 3A4 and resid 397 and name CA)	10.34	0.42	0.42
	assign (segid 3A4 and resid 133 and name CA)	(segid 3A4 and resid 397 and name CB)	11.21	0.52	0.51
	assign (segid 3A4 and resid 133 and name CA)	(segid 3A4 and resid 398 and name CA)	13.17	0.43	0.44
	assign (segid 3A4 and resid 133 and name CA)	(segid 3A4 and resid 398 and name CB)	14.37	0.40	0.40
50	assign (segid 3A4 and resid 133 and name CA)	(segid 3A4 and resid 399 and name CA)	11.66	0.64	0.64
	assign (segid 3A4 and resid 133 and name CA)	(segid 3A4 and resid 399 and name CB)	11.09	0.62	0.62
	assign (segid 3A4 and resid 133 and name CA)	(segid 3A4 and resid 400 and name CA)	9.27	0.82	0.82
	assign (segid 3A4 and resid 133 and name CA)	(segid 3A4 and resid 400 and name CB)	8.17	0.84	0.84
	assign (segid 3A4 and resid 133 and name CA)	(segid 3A4 and resid 401 and name CA)	12.38	0.84	0.84
55	assign (segid 3A4 and resid 133 and name CA)	(segid 3A4 and resid 402 and name CA)	14.69	0.88	0.88
	assign (segid 3A4 and resid 133 and name CA)	(segid 3A4 and resid 402 and name CB)	15.14	0.88	0.88
	assign (segid 3A4 and resid 133 and name CA)	(segid 3A4 and resid 403 and name CA)	13.08	1.04	1.03
	assign (segid 3A4 and resid 133 and name CA)	(segid 3A4 and resid 403 and name CB)	11.87	1.08	1.08
	assign (segid 3A4 and resid 133 and name CA)	(segid 3A4 and resid 404 and name CA)	12.81	0.94	0.93
60	assign (segid 3A4 and resid 133 and name CA)	(segid 3A4 and resid 404 and name CB)	12.10	0.85	0.85
	assign (segid 3A4 and resid 133 and name CA)	(segid 3A4 and resid 405 and name CA)	16.24	0.80	0.80
	assign (segid 3A4 and resid 133 and name CA)	(segid 3A4 and resid 405 and name CB)	16.75	0.74	0.75
	assign (segid 3A4 and resid 133 and name CA)	(segid 3A4 and resid 406 and name CA)	17.78	1.01	1.01
	assign (segid 3A4 and resid 133 and name CA)	(segid 3A4 and resid 407 and name CA)	16.86	1.16	1.17
65	assign (segid 3A4 and resid 133 and name CA)	(segid 3A4 and resid 407 and name CB)	15.61	1.25	1.24
	assign (segid 3A4 and resid 133 and name CA)	(segid 3A4 and resid 408 and name CA)	17.77	1.04	1.04
	assign (segid 3A4 and resid 133 and name CA)	(segid 3A4 and resid 408 and name CB)	17.34	1.01	1.02
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 133 and name CG1)	1.54	0.02	0.03
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 133 and name CG2)	1.53	0.01	0.02
70	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 134 and name C)	5.45	0.04	0.03
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 134 and name CA)	4.52	0.05	0.04
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 134 and name N)	3.19	0.06	0.05
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 134 and name O)	6.31	0.08	0.08
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 135 and name C)	6.91	0.10	0.10
75	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 135 and name CA)	6.82	0.07	0.07
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 135 and name CB)	7.34	0.11	0.11
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 135 and name N)	5.61	0.03	0.03
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 136 and name C)	6.81	0.21	0.20
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 136 and name CA)	6.52	0.12	0.11
80	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 136 and name CB)	5.88	0.21	0.21
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 136 and name N)	6.02	0.11	0.11
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 137 and name CA)	6.80	0.34	0.35

	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 137 and name N)	6.13	0.22	0.22
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 138 and name CA)	9.46	0.30	0.30
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 138 and name CB)	9.51	0.29	0.28
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 139 and name CA)	10.85	0.45	0.45
5	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 140 and name CA)	11.12	0.48	0.48
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 140 and name CB)	10.90	0.49	0.49
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 141 and name CA)	11.97	1.07	1.06
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 141 and name CB)	13.19	1.41	1.40
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 147 and name CA)	13.63	1.88	1.88
10	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 147 and name CB)	14.23	2.33	2.33
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 148 and name CA)	14.97	0.90	0.90
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 149 and name CA)	13.71	1.20	1.21
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 149 and name CB)	13.60	1.28	1.28
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 150 and name CA)	12.86	1.08	1.08
15	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 151 and name CA)	14.79	0.94	0.95
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 152 and name CA)	15.02	1.86	1.86
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 152 and name CB)	15.04	2.54	2.55
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 153 and name CA)	13.60	1.18	1.18
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 153 and name CB)	12.97	1.01	1.00
20	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 154 and name CA)	14.32	1.43	1.43
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 155 and name CA)	16.61	1.28	1.27
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 155 and name CB)	17.08	1.57	1.58
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 156 and name CA)	16.21	2.10	2.10
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 156 and name CB)	15.59	2.51	2.52
25	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 157 and name CA)	15.60	1.45	1.46
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 157 and name CB)	14.66	1.65	1.65
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 194 and name CB)	16.62	2.33	2.32
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 197 and name CB)	16.81	2.23	2.22
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 198 and name CA)	16.30	2.38	2.39
30	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 198 and name CB)	15.91	2.44	2.45
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 201 and name CA)	17.21	1.81	1.80
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 201 and name CB)	15.77	1.84	1.85
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 205 and name CB)	17.87	1.27	1.28
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 219 and name CA)	12.00	0.72	0.72
35	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 219 and name CB)	11.67	0.84	0.85
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 220 and name CA)	11.85	1.03	1.02
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 220 and name CB)	10.77	1.11	1.11
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 221 and name CA)	13.94	1.20	1.20
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 221 and name CB)	13.77	1.20	1.19
40	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 222 and name CA)	16.51	0.99	1.00
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 222 and name CB)	16.50	0.83	0.83
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 223 and name CA)	16.82	0.97	0.98
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 223 and name CB)	15.90	0.89	0.89
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 224 and name CA)	17.45	1.26	1.26
45	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 224 and name CB)	16.61	1.32	1.32
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 247 and name CA)	15.46	2.55	2.55
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 247 and name CB)	15.76	2.46	2.47
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 248 and name CA)	12.84	2.67	2.66
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 248 and name CB)	13.27	2.64	2.63
50	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 249 and name CA)	13.61	2.62	2.61
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 250 and name CA)	13.43	2.31	2.31
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 250 and name CB)	14.39	2.25	2.25
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 251 and name CA)	10.05	2.28	2.29
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 251 and name CB)	9.78	2.41	2.41
55	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 252 and name CA)	8.87	2.32	2.31
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 252 and name CB)	9.62	2.42	2.41
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 253 and name CA)	11.37	1.80	1.80
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 254 and name CA)	11.34	1.48	1.48
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 255 and name CA)	8.23	1.54	1.54
60	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 256 and name CA)	8.07	1.27	1.26
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 257 and name CA)	11.44	0.96	0.95
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 258 and name CA)	12.05	0.60	0.60
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 258 and name CB)	12.11	0.73	0.73
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 259 and name CA)	9.76	0.36	0.36
65	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 259 and name CB)	8.37	0.40	0.39
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 260 and name CA)	10.86	0.31	0.32
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 260 and name CB)	10.96	0.36	0.35
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 261 and name CA)	14.25	0.33	0.33
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 262 and name CA)	14.29	0.51	0.51
70	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 262 and name CB)	13.59	0.57	0.56
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 263 and name CA)	13.52	0.84	0.83
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 263 and name CB)	12.33	0.89	0.89
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 264 and name CA)	16.13	0.59	0.60
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 265 and name CA)	18.48	0.56	0.56
75	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 266 and name CA)	18.21	0.88	0.88
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 309 and name CB)	16.64	1.46	1.45
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 313 and name CA)	18.59	0.91	0.91
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 313 and name CB)	17.85	0.92	0.91
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 318 and name CB)	16.80	1.03	1.02
80	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 319 and name CB)	18.11	1.13	1.14
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 384 and name CA)	17.53	0.59	0.58
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 384 and name CB)	16.99	0.57	0.57
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 391 and name CA)	15.56	1.00	1.00

	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 391 and name CB)	14.92	0.91	0.91
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 392 and name CA)	14.12	1.01	1.02
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 392 and name CB)	14.08	1.18	1.18
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 393 and name CA)	10.84	0.73	0.73
5	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 394 and name CA)	12.91	0.34	0.34
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 394 and name CB)	14.38	0.36	0.36
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 395 and name CA)	12.42	0.40	0.41
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 396 and name CA)	8.81	0.55	0.56
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 396 and name CB)	7.99	0.35	0.35
10	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 397 and name CA)	9.35	0.52	0.51
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 397 and name CB)	10.19	0.44	0.43
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 398 and name CA)	12.16	0.84	0.84
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 398 and name CB)	13.37	0.77	0.76
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 399 and name CA)	10.80	1.29	1.30
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 399 and name CB)	10.33	1.28	1.28
15	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 400 and name CA)	8.37	1.46	1.45
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 401 and name CA)	7.23	1.40	1.39
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 402 and name CA)	11.38	1.30	1.30
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 402 and name CB)	13.78	1.49	1.49
20	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 402 and name CB)	14.23	1.50	1.51
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 403 and name CA)	12.37	1.74	1.74
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 403 and name CB)	11.22	1.82	1.82
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 404 and name CA)	12.10	1.51	1.51
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 404 and name CB)	11.36	1.35	1.34
25	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 405 and name CA)	15.41	1.28	1.29
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 405 and name CB)	15.86	1.20	1.19
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 406 and name CA)	17.06	1.61	1.61
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 407 and name CA)	16.35	1.77	1.78
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 407 and name CB)	15.16	1.87	1.86
30	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 408 and name CB)	16.72	1.52	1.52
	assign (segid 3A4 and resid 133 and name CB)	(segid 3A4 and resid 134 and name C)	6.80	0.04	0.04
	assign (segid 3A4 and resid 133 and name CG1)	(segid 3A4 and resid 134 and name CA)	5.98	0.04	0.04
	assign (segid 3A4 and resid 133 and name CG1)	(segid 3A4 and resid 134 and name N)	4.59	0.03	0.04
	assign (segid 3A4 and resid 133 and name CG1)	(segid 3A4 and resid 134 and name O)	7.68	0.08	0.09
35	assign (segid 3A4 and resid 133 and name CG1)	(segid 3A4 and resid 135 and name CA)	7.89	0.09	0.09
	assign (segid 3A4 and resid 133 and name CG1)	(segid 3A4 and resid 135 and name N)	6.80	0.05	0.05
	assign (segid 3A4 and resid 133 and name CG1)	(segid 3A4 and resid 136 and name CA)	7.24	0.19	0.18
	assign (segid 3A4 and resid 133 and name CG1)	(segid 3A4 and resid 136 and name CB)	6.33	0.25	0.24
	assign (segid 3A4 and resid 133 and name CG1)	(segid 3A4 and resid 136 and name N)	6.88	0.15	0.15
40	assign (segid 3A4 and resid 133 and name CG1)	(segid 3A4 and resid 137 and name N)	7.17	0.28	0.29
	assign (segid 3A4 and resid 133 and name CG2)	(segid 3A4 and resid 134 and name C)	5.68	0.08	0.09
	assign (segid 3A4 and resid 133 and name CG2)	(segid 3A4 and resid 134 and name CA)	4.70	0.12	0.12
	assign (segid 3A4 and resid 133 and name CG2)	(segid 3A4 and resid 134 and name N)	3.68	0.12	0.12
	assign (segid 3A4 and resid 133 and name CG2)	(segid 3A4 and resid 134 and name O)	6.31	0.13	0.13
45	assign (segid 3A4 and resid 133 and name CG2)	(segid 3A4 and resid 135 and name C)	7.26	0.15	0.15
	assign (segid 3A4 and resid 133 and name CG2)	(segid 3A4 and resid 135 and name CA)	7.34	0.11	0.12
	assign (segid 3A4 and resid 133 and name CG2)	(segid 3A4 and resid 135 and name N)	6.15	0.07	0.06
	assign (segid 3A4 and resid 133 and name CG2)	(segid 3A4 and resid 136 and name C)	6.61	0.25	0.26
	assign (segid 3A4 and resid 133 and name CG2)	(segid 3A4 and resid 136 and name CA)	6.66	0.17	0.16
50	assign (segid 3A4 and resid 133 and name CG2)	(segid 3A4 and resid 136 and name CB)	6.06	0.21	0.20
	assign (segid 3A4 and resid 133 and name CG2)	(segid 3A4 and resid 136 and name N)	6.36	0.17	0.17
	assign (segid 3A4 and resid 133 and name CG2)	(segid 3A4 and resid 136 and name O)	7.55	0.37	0.37
	assign (segid 3A4 and resid 133 and name CG2)	(segid 3A4 and resid 137 and name C)	7.49	0.43	0.42
	assign (segid 3A4 and resid 133 and name CG2)	(segid 3A4 and resid 137 and name CA)	6.16	0.37	0.37
55	assign (segid 3A4 and resid 133 and name CG2)	(segid 3A4 and resid 137 and name N)	5.79	0.22	0.22
	assign (segid 3A4 and resid 133 and name N)	(segid 3A4 and resid 133 and name C)	2.45	0.02	0.02
	assign (segid 3A4 and resid 133 and name N)	(segid 3A4 and resid 133 and name CA)	1.45	0.00	0.00
	assign (segid 3A4 and resid 133 and name N)	(segid 3A4 and resid 133 and name CB)	2.47	0.02	0.02
	assign (segid 3A4 and resid 133 and name N)	(segid 3A4 and resid 133 and name CG1)	2.99	0.05	0.04
60	assign (segid 3A4 and resid 133 and name N)	(segid 3A4 and resid 133 and name CG2)	3.83	0.03	0.02
	assign (segid 3A4 and resid 133 and name N)	(segid 3A4 and resid 133 and name O)	3.47	0.04	0.04
	assign (segid 3A4 and resid 133 and name N)	(segid 3A4 and resid 134 and name C)	4.67	0.07	0.07
	assign (segid 3A4 and resid 133 and name N)	(segid 3A4 and resid 134 and name CA)	4.22	0.05	0.05
	assign (segid 3A4 and resid 133 and name N)	(segid 3A4 and resid 134 and name N)	2.82	0.07	0.07
65	assign (segid 3A4 and resid 133 and name N)	(segid 3A4 and resid 134 and name O)	5.75	0.09	0.08
	assign (segid 3A4 and resid 133 and name N)	(segid 3A4 and resid 135 and name C)	5.57	0.07	0.07
	assign (segid 3A4 and resid 133 and name N)	(segid 3A4 and resid 135 and name CA)	5.26	0.07	0.08
	assign (segid 3A4 and resid 133 and name N)	(segid 3A4 and resid 135 and name CB)	5.38	0.15	0.14
	assign (segid 3A4 and resid 133 and name N)	(segid 3A4 and resid 135 and name N)	4.25	0.06	0.07
70	assign (segid 3A4 and resid 133 and name N)	(segid 3A4 and resid 135 and name O)	6.77	0.08	0.08
	assign (segid 3A4 and resid 133 and name N)	(segid 3A4 and resid 136 and name C)	6.38	0.16	0.17
	assign (segid 3A4 and resid 133 and name N)	(segid 3A4 and resid 136 and name CA)	5.61	0.09	0.10
	assign (segid 3A4 and resid 133 and name N)	(segid 3A4 and resid 136 and name CB)	5.13	0.19	0.19
	assign (segid 3A4 and resid 133 and name N)	(segid 3A4 and resid 136 and name N)	4.79	0.07	0.06
75	assign (segid 3A4 and resid 133 and name N)	(segid 3A4 and resid 136 and name O)	7.53	0.18	0.19
	assign (segid 3A4 and resid 133 and name N)	(segid 3A4 and resid 137 and name CA)	7.08	0.29	0.29
	assign (segid 3A4 and resid 133 and name N)	(segid 3A4 and resid 137 and name N)	6.00	0.21	0.21
	assign (segid 3A4 and resid 133 and name O)	(segid 3A4 and resid 133 and name CB)	3.32	0.09	0.09
	assign (segid 3A4 and resid 133 and name O)	(segid 3A4 and resid 133 and name CG1)	4.56	0.06	0.06
80	assign (segid 3A4 and resid 133 and name O)	(segid 3A4 and resid 133 and name CG2)	3.24	0.14	0.14
	assign (segid 3A4 and resid 133 and name O)	(segid 3A4 and resid 134 and name C)	2.96	0.05	0.06
	assign (segid 3A4 and resid 133 and name O)	(segid 3A4 and resid 134 and name CA)	2.75	0.03	0.03
	assign (segid 3A4 and resid 133 and name O)	(segid 3A4 and resid 134 and name N)	2.25	0.02	0.01

	assign (segid 3A4 and resid 133 and name O)	(segid 3A4 and resid 134 and name O)	3.42	0.09	0.09
	assign (segid 3A4 and resid 133 and name O)	(segid 3A4 and resid 135 and name C)	4.13	0.10	0.10
	assign (segid 3A4 and resid 133 and name O)	(segid 3A4 and resid 135 and name CA)	4.39	0.10	0.10
	assign (segid 3A4 and resid 133 and name O)	(segid 3A4 and resid 135 and name CB)	5.41	0.15	0.14
	assign (segid 3A4 and resid 133 and name O)	(segid 3A4 and resid 135 and name N)	3.42	0.09	0.09
5	assign (segid 3A4 and resid 133 and name O)	(segid 3A4 and resid 135 and name O)	5.02	0.15	0.14
	assign (segid 3A4 and resid 133 and name O)	(segid 3A4 and resid 136 and name C)	3.80	0.08	0.08
	assign (segid 3A4 and resid 133 and name O)	(segid 3A4 and resid 136 and name CA)	3.83	0.14	0.15
	assign (segid 3A4 and resid 133 and name O)	(segid 3A4 and resid 136 and name CB)	3.81	0.37	0.37
	assign (segid 3A4 and resid 133 and name O)	(segid 3A4 and resid 136 and name N)	3.36	0.10	0.10
10	assign (segid 3A4 and resid 133 and name O)	(segid 3A4 and resid 136 and name O)	4.92	0.08	0.08
	assign (segid 3A4 and resid 133 and name O)	(segid 3A4 and resid 137 and name C)	4.87	0.27	0.27
	assign (segid 3A4 and resid 133 and name O)	(segid 3A4 and resid 137 and name CA)	3.73	0.24	0.25
	assign (segid 3A4 and resid 133 and name O)	(segid 3A4 and resid 137 and name N)	2.95	0.14	0.13
	assign (segid 3A4 and resid 133 and name O)	(segid 3A4 and resid 137 and name O)	5.99	0.27	0.27
15	assign (segid 3A4 and resid 133 and name O)	(segid 3A4 and resid 138 and name C)	7.04	0.33	0.32
	assign (segid 3A4 and resid 133 and name O)	(segid 3A4 and resid 138 and name CA)	6.24	0.25	0.25
	assign (segid 3A4 and resid 133 and name O)	(segid 3A4 and resid 138 and name CB)	6.48	0.21	0.20
	assign (segid 3A4 and resid 133 and name O)	(segid 3A4 and resid 138 and name N)	4.90	0.26	0.25
	assign (segid 3A4 and resid 133 and name O)	(segid 3A4 and resid 139 and name N)	6.63	0.33	0.33
20	assign (segid 3A4 and resid 133 and name O)	(segid 3A4 and resid 134 and name O)	1.24	0.01	0.01
	assign (segid 3A4 and resid 134 and name C)	(segid 3A4 and resid 135 and name C)	3.04	0.05	0.05
	assign (segid 3A4 and resid 134 and name C)	(segid 3A4 and resid 135 and name CA)	2.44	0.02	0.01
	assign (segid 3A4 and resid 134 and name C)	(segid 3A4 and resid 135 and name CB)	3.71	0.02	0.02
	assign (segid 3A4 and resid 134 and name C)	(segid 3A4 and resid 135 and name N)	1.33	0.01	0.00
25	assign (segid 3A4 and resid 134 and name C)	(segid 3A4 and resid 135 and name O)	3.85	0.07	0.07
	assign (segid 3A4 and resid 134 and name C)	(segid 3A4 and resid 136 and name C)	4.56	0.14	0.14
	assign (segid 3A4 and resid 134 and name C)	(segid 3A4 and resid 136 and name CA)	4.50	0.14	0.15
	assign (segid 3A4 and resid 134 and name C)	(segid 3A4 and resid 136 and name CB)	5.32	0.26	0.25
	assign (segid 3A4 and resid 134 and name C)	(segid 3A4 and resid 136 and name N)	3.33	0.15	0.15
30	assign (segid 3A4 and resid 134 and name C)	(segid 3A4 and resid 136 and name O)	5.66	0.16	0.16
	assign (segid 3A4 and resid 134 and name C)	(segid 3A4 and resid 137 and name C)	4.82	0.03	0.03
	assign (segid 3A4 and resid 134 and name C)	(segid 3A4 and resid 137 and name CA)	4.51	0.07	0.08
	assign (segid 3A4 and resid 134 and name C)	(segid 3A4 and resid 137 and name N)	3.77	0.09	0.10
	assign (segid 3A4 and resid 134 and name C)	(segid 3A4 and resid 137 and name O)	6.03	0.03	0.03
35	assign (segid 3A4 and resid 134 and name C)	(segid 3A4 and resid 138 and name C)	5.66	0.36	0.36
	assign (segid 3A4 and resid 134 and name C)	(segid 3A4 and resid 138 and name CA)	4.96	0.08	0.07
	assign (segid 3A4 and resid 134 and name C)	(segid 3A4 and resid 138 and name CB)	4.72	0.33	0.32
	assign (segid 3A4 and resid 134 and name C)	(segid 3A4 and resid 138 and name N)	4.08	0.04	0.03
	assign (segid 3A4 and resid 134 and name C)	(segid 3A4 and resid 138 and name O)	6.71	0.43	0.42
40	assign (segid 3A4 and resid 134 and name C)	(segid 3A4 and resid 139 and name C)	6.55	0.85	0.86
	assign (segid 3A4 and resid 134 and name C)	(segid 3A4 and resid 139 and name CA)	6.38	0.77	0.76
	assign (segid 3A4 and resid 134 and name C)	(segid 3A4 and resid 139 and name N)	5.37	0.55	0.54
	assign (segid 3A4 and resid 134 and name C)	(segid 3A4 and resid 140 and name C)	6.36	0.81	0.80
	assign (segid 3A4 and resid 134 and name C)	(segid 3A4 and resid 140 and name CB)	6.08	0.51	0.52
45	assign (segid 3A4 and resid 134 and name C)	(segid 3A4 and resid 140 and name N)	5.75	0.80	0.80
	assign (segid 3A4 and resid 134 and name C)	(segid 3A4 and resid 140 and name O)	5.68	1.38	1.37
	assign (segid 3A4 and resid 134 and name C)	(segid 3A4 and resid 134 and name C)	1.53	0.02	0.01
	assign (segid 3A4 and resid 134 and name CA)	(segid 3A4 and resid 134 and name O)	2.41	0.02	0.01
	assign (segid 3A4 and resid 134 and name CA)	(segid 3A4 and resid 135 and name C)	4.43	0.03	0.04
50	assign (segid 3A4 and resid 134 and name CA)	(segid 3A4 and resid 135 and name CA)	3.82	0.03	0.03
	assign (segid 3A4 and resid 134 and name CA)	(segid 3A4 and resid 135 and name CB)	4.88	0.05	0.05
	assign (segid 3A4 and resid 134 and name CA)	(segid 3A4 and resid 135 and name N)	2.45	0.04	0.03
	assign (segid 3A4 and resid 134 and name CA)	(segid 3A4 and resid 135 and name O)	5.31	0.07	0.07
	assign (segid 3A4 and resid 134 and name CA)	(segid 3A4 and resid 136 and name C)	5.48	0.15	0.15
55	assign (segid 3A4 and resid 134 and name CA)	(segid 3A4 and resid 136 and name CA)	5.50	0.16	0.15
	assign (segid 3A4 and resid 134 and name CA)	(segid 3A4 and resid 136 and name CB)	6.00	0.32	0.31
	assign (segid 3A4 and resid 134 and name CA)	(segid 3A4 and resid 136 and name N)	4.43	0.13	0.14
	assign (segid 3A4 and resid 134 and name CA)	(segid 3A4 and resid 136 and name O)	6.61	0.15	0.15
	assign (segid 3A4 and resid 134 and name CA)	(segid 3A4 and resid 137 and name C)	5.58	0.06	0.05
60	assign (segid 3A4 and resid 134 and name CA)	(segid 3A4 and resid 137 and name CA)	5.04	0.12	0.12
	assign (segid 3A4 and resid 134 and name CA)	(segid 3A4 and resid 137 and name N)	4.50	0.14	0.13
	assign (segid 3A4 and resid 134 and name CA)	(segid 3A4 and resid 137 and name O)	6.75	0.05	0.05
	assign (segid 3A4 and resid 134 and name CA)	(segid 3A4 and resid 138 and name C)	6.86	0.42	0.42
	assign (segid 3A4 and resid 134 and name CA)	(segid 3A4 and resid 138 and name CA)	5.98	0.14	0.13
65	assign (segid 3A4 and resid 134 and name CA)	(segid 3A4 and resid 138 and name CB)	5.67	0.25	0.26
	assign (segid 3A4 and resid 134 and name CA)	(segid 3A4 and resid 138 and name N)	5.03	0.09	0.09
	assign (segid 3A4 and resid 134 and name CA)	(segid 3A4 and resid 139 and name CA)	7.77	0.76	0.77
	assign (segid 3A4 and resid 134 and name CA)	(segid 3A4 and resid 139 and name N)	6.70	0.57	0.56
	assign (segid 3A4 and resid 134 and name CA)	(segid 3A4 and resid 140 and name CA)	7.65	1.05	1.05
70	assign (segid 3A4 and resid 134 and name CA)	(segid 3A4 and resid 140 and name CB)	7.25	0.81	0.81
	assign (segid 3A4 and resid 134 and name CA)	(segid 3A4 and resid 141 and name CA)	9.33	1.90	1.90
	assign (segid 3A4 and resid 134 and name CA)	(segid 3A4 and resid 141 and name CB)	10.60	2.08	2.07
	assign (segid 3A4 and resid 134 and name CA)	(segid 3A4 and resid 141 and name N)	12.18	1.33	1.34
	assign (segid 3A4 and resid 134 and name CA)	(segid 3A4 and resid 147 and name CB)	13.04	1.55	1.56
75	assign (segid 3A4 and resid 134 and name CA)	(segid 3A4 and resid 148 and name CA)	13.26	1.07	1.06
	assign (segid 3A4 and resid 134 and name CA)	(segid 3A4 and resid 149 and name CA)	11.64	0.98	0.98
	assign (segid 3A4 and resid 134 and name CA)	(segid 3A4 and resid 149 and name CB)	11.26	0.99	1.00
	assign (segid 3A4 and resid 134 and name CA)	(segid 3A4 and resid 150 and name CA)	11.33	1.21	1.20
	assign (segid 3A4 and resid 134 and name CA)	(segid 3A4 and resid 151 and name CA)	13.48	0.72	0.72
80	assign (segid 3A4 and resid 134 and name CA)	(segid 3A4 and resid 152 and name CA)	13.30	1.21	1.21
	assign (segid 3A4 and resid 134 and name CA)	(segid 3A4 and resid 152 and name CB)	13.15	1.90	1.90
	assign (segid 3A4 and resid 134 and name CA)	(segid 3A4 and resid 153 and name CA)	11.85	1.13	1.14

	assign (segid 3A4 and resid 134 and name CA) (segid 3A4 and resid 153 and name CB)	11.09	1.42	1.42
	assign (segid 3A4 and resid 134 and name CA) (segid 3A4 and resid 151 and name CA)	13.10	2.03	2.03
	assign (segid 3A4 and resid 134 and name CA) (segid 3A4 and resid 155 and name CA)	15.40	1.04	1.03
	assign (segid 3A4 and resid 134 and name CA) (segid 3A4 and resid 155 and name CB)	15.81	0.91	0.90
5	assign (segid 3A4 and resid 134 and name CA) (segid 3A4 and resid 156 and name CA)	14.80	1.37	1.37
	assign (segid 3A4 and resid 134 and name CA) (segid 3A4 and resid 156 and name CB)	14.05	1.52	1.52
	assign (segid 3A4 and resid 134 and name CA) (segid 3A4 and resid 157 and name CA)	14.34	2.31	2.31
	assign (segid 3A4 and resid 134 and name CA) (segid 3A4 and resid 157 and name CB)	13.36	2.76	2.75
	assign (segid 3A4 and resid 134 and name CA) (segid 3A4 and resid 191 and name CA)	18.01	0.96	0.96
10	assign (segid 3A4 and resid 134 and name CA) (segid 3A4 and resid 191 and name CB)	18.88	0.82	0.82
	assign (segid 3A4 and resid 134 and name CA) (segid 3A4 and resid 194 and name CA)	14.28	1.31	1.31
	assign (segid 3A4 and resid 134 and name CA) (segid 3A4 and resid 194 and name CB)	13.83	1.11	1.10
	assign (segid 3A4 and resid 134 and name CA) (segid 3A4 and resid 195 and name CA)	15.94	1.25	1.25
	assign (segid 3A4 and resid 134 and name CA) (segid 3A4 and resid 195 and name CB)	17.18	1.14	1.14
15	assign (segid 3A4 and resid 134 and name CA) (segid 3A4 and resid 196 and name CA)	17.34	1.62	1.62
	assign (segid 3A4 and resid 134 and name CA) (segid 3A4 and resid 197 and name CA)	14.25	1.70	1.70
	assign (segid 3A4 and resid 134 and name CA) (segid 3A4 and resid 197 and name CB)	13.36	1.69	1.69
	assign (segid 3A4 and resid 134 and name CA) (segid 3A4 and resid 198 and name CA)	12.74	1.56	1.56
	assign (segid 3A4 and resid 134 and name CA) (segid 3A4 and resid 198 and name CB)	12.47	1.38	1.39
20	assign (segid 3A4 and resid 134 and name CA) (segid 3A4 and resid 199 and name CA)	16.18	1.56	1.57
	assign (segid 3A4 and resid 134 and name CA) (segid 3A4 and resid 199 and name CB)	17.44	1.54	1.55
	assign (segid 3A4 and resid 134 and name CA) (segid 3A4 and resid 200 and name CA)	16.53	1.71	1.72
	assign (segid 3A4 and resid 134 and name CA) (segid 3A4 and resid 201 and name CA)	13.50	1.61	1.61
	assign (segid 3A4 and resid 134 and name CA) (segid 3A4 and resid 201 and name CB)	12.04	1.63	1.63
25	assign (segid 3A4 and resid 134 and name CA) (segid 3A4 and resid 202 and name CA)	14.94	1.33	1.33
	assign (segid 3A4 and resid 134 and name CA) (segid 3A4 and resid 202 and name CB)	15.31	1.29	1.29
	assign (segid 3A4 and resid 134 and name CA) (segid 3A4 and resid 204 and name CA)	17.43	1.36	1.37
	assign (segid 3A4 and resid 134 and name CA) (segid 3A4 and resid 204 and name CB)	16.61	1.32	1.33
30	assign (segid 3A4 and resid 134 and name CA) (segid 3A4 and resid 205 and name CA)	15.81	1.20	1.20
	assign (segid 3A4 and resid 134 and name CA) (segid 3A4 and resid 205 and name CB)	14.56	1.11	1.11
	assign (segid 3A4 and resid 134 and name CA) (segid 3A4 and resid 219 and name CA)	10.04	0.33	0.33
	assign (segid 3A4 and resid 134 and name CA) (segid 3A4 and resid 219 and name CB)	9.40	0.57	0.58
	assign (segid 3A4 and resid 134 and name CA) (segid 3A4 and resid 220 and name CA)	9.75	0.16	0.17
	assign (segid 3A4 and resid 134 and name CA) (segid 3A4 and resid 220 and name CB)	8.73	0.28	0.28
35	assign (segid 3A4 and resid 134 and name CA) (segid 3A4 and resid 221 and name CA)	11.06	0.33	0.33
	assign (segid 3A4 and resid 134 and name CA) (segid 3A4 and resid 221 and name CB)	10.64	0.48	0.48
	assign (segid 3A4 and resid 134 and name CA) (segid 3A4 and resid 222 and name CA)	13.88	0.39	0.39
	assign (segid 3A4 and resid 134 and name CA) (segid 3A4 and resid 222 and name CB)	13.99	0.40	0.41
	assign (segid 3A4 and resid 134 and name CA) (segid 3A4 and resid 223 and name CA)	14.73	0.12	0.13
40	assign (segid 3A4 and resid 134 and name CA) (segid 3A4 and resid 223 and name CB)	14.07	0.22	0.22
	assign (segid 3A4 and resid 134 and name CA) (segid 3A4 and resid 224 and name CA)	15.03	0.25	0.25
	assign (segid 3A4 and resid 134 and name CA) (segid 3A4 and resid 224 and name CB)	14.08	0.29	0.28
	assign (segid 3A4 and resid 134 and name CA) (segid 3A4 and resid 225 and name CA)	16.98	0.35	0.35
	assign (segid 3A4 and resid 134 and name CA) (segid 3A4 and resid 225 and name CB)	16.64	0.42	0.43
45	assign (segid 3A4 and resid 134 and name CA) (segid 3A4 and resid 226 and name CA)	19.36	0.25	0.26
	assign (segid 3A4 and resid 134 and name CA) (segid 3A4 and resid 244 and name CA)	15.69	0.88	0.89
	assign (segid 3A4 and resid 134 and name CA) (segid 3A4 and resid 244 and name CB)	15.96	0.99	0.98
	assign (segid 3A4 and resid 134 and name CA) (segid 3A4 and resid 245 and name CA)	14.70	1.18	1.19
	assign (segid 3A4 and resid 134 and name CA) (segid 3A4 and resid 245 and name CB)	15.76	1.28	1.28
50	assign (segid 3A4 and resid 134 and name CA) (segid 3A4 and resid 246 and name CA)	15.27	0.86	0.85
	assign (segid 3A4 and resid 134 and name CA) (segid 3A4 and resid 246 and name CB)	16.64	0.84	0.85
	assign (segid 3A4 and resid 134 and name CA) (segid 3A4 and resid 247 and name CA)	13.20	0.65	0.66
	assign (segid 3A4 and resid 134 and name CA) (segid 3A4 and resid 247 and name CB)	13.52	0.57	0.57
	assign (segid 3A4 and resid 134 and name CA) (segid 3A4 and resid 248 and name CA)	10.16	0.85	0.85
55	assign (segid 3A4 and resid 134 and name CA) (segid 3A4 and resid 248 and name CB)	10.31	1.05	1.04
	assign (segid 3A4 and resid 134 and name CA) (segid 3A4 and resid 249 and name CA)	11.12	0.79	0.78
	assign (segid 3A4 and resid 134 and name CA) (segid 3A4 and resid 250 and name CA)	11.68	0.53	0.53
	assign (segid 3A4 and resid 134 and name CA) (segid 3A4 and resid 250 and name CB)	12.71	0.56	0.57
	assign (segid 3A4 and resid 134 and name CA) (segid 3A4 and resid 251 and name CA)	8.56	0.65	0.64
60	assign (segid 3A4 and resid 134 and name CA) (segid 3A4 and resid 251 and name CB)	8.12	0.57	0.56
	assign (segid 3A4 and resid 134 and name CA) (segid 3A4 and resid 252 and name CA)	7.06	0.64	0.63
	assign (segid 3A4 and resid 134 and name CA) (segid 3A4 and resid 252 and name CB)	7.41	0.64	0.64
	assign (segid 3A4 and resid 134 and name CA) (segid 3A4 and resid 253 and name CA)	10.12	0.79	0.78
	assign (segid 3A4 and resid 134 and name CA) (segid 3A4 and resid 254 and name CA)	10.83	1.24	1.23
65	assign (segid 3A4 and resid 134 and name CA) (segid 3A4 and resid 255 and name CA)	8.18	1.69	1.68
	assign (segid 3A4 and resid 134 and name CA) (segid 3A4 and resid 256 and name CA)	8.18	1.00	1.00
	assign (segid 3A4 and resid 134 and name CA) (segid 3A4 and resid 257 and name CA)	11.83	1.03	1.03
	assign (segid 3A4 and resid 134 and name CA) (segid 3A4 and resid 258 and name CA)	13.11	1.32	1.31
	assign (segid 3A4 and resid 134 and name CA) (segid 3A4 and resid 258 and name CB)	13.09	1.36	1.35
70	assign (segid 3A4 and resid 134 and name CA) (segid 3A4 and resid 259 and name CA)	11.60	1.28	1.27
	assign (segid 3A4 and resid 134 and name CA) (segid 3A4 and resid 259 and name CB)	10.28	1.28	1.29
	assign (segid 3A4 and resid 134 and name CA) (segid 3A4 and resid 260 and name CA)	12.53	0.99	0.98
	assign (segid 3A4 and resid 134 and name CA) (segid 3A4 and resid 260 and name CB)	12.24	0.84	0.85
	assign (segid 3A4 and resid 134 and name CA) (segid 3A4 and resid 261 and name CA)	15.88	1.03	1.03
75	assign (segid 3A4 and resid 134 and name CA) (segid 3A4 and resid 262 and name CA)	16.47	1.22	1.21
	assign (segid 3A4 and resid 134 and name CA) (segid 3A4 and resid 262 and name CB)	15.80	1.29	1.30
	assign (segid 3A4 and resid 134 and name CA) (segid 3A4 and resid 263 and name CA)	16.08	1.08	1.08
	assign (segid 3A4 and resid 134 and name CA) (segid 3A4 and resid 263 and name CB)	14.92	1.02	1.01
	assign (segid 3A4 and resid 134 and name CA) (segid 3A4 and resid 391 and name CA)	16.17	1.30	1.29
80	assign (segid 3A4 and resid 134 and name CA) (segid 3A4 and resid 391 and name CB)	15.75	1.33	1.33
	assign (segid 3A4 and resid 134 and name CA) (segid 3A4 and resid 392 and name CA)	14.42	1.25	1.26
	assign (segid 3A4 and resid 134 and name CA) (segid 3A4 and resid 392 and name CB)	14.04	1.22	1.21
	assign (segid 3A4 and resid 134 and name CA) (segid 3A4 and resid 393 and name CA)	11.59	1.35	1.35

	assign (segid 3A4 and resid 134 and name CA)	(segid 3A4 and resid 394 and name CA)	14.44	1.46	1.46
	assign (segid 3A4 and resid 134 and name CA)	(segid 3A4 and resid 394 and name CB)	15.88	1.44	1.44
	assign (segid 3A4 and resid 134 and name CA)	(segid 3A4 and resid 395 and name CA)	14.30	1.37	1.38
	assign (segid 3A4 and resid 134 and name CA)	(segid 3A4 and resid 396 and name CA)	10.73	1.40	1.40
	assign (segid 3A4 and resid 134 and name CA)	(segid 3A4 and resid 396 and name CB)	9.48	1.40	1.41
5	assign (segid 3A4 and resid 134 and name CA)	(segid 3A4 and resid 397 and name CA)	11.58	1.37	1.37
	assign (segid 3A4 and resid 134 and name CA)	(segid 3A4 and resid 397 and name CB)	12.20	1.34	1.34
	assign (segid 3A4 and resid 134 and name CA)	(segid 3A4 and resid 398 and name CA)	14.86	1.36	1.37
	assign (segid 3A4 and resid 134 and name CA)	(segid 3A4 and resid 398 and name CB)	15.98	1.36	1.37
	assign (segid 3A4 and resid 134 and name CA)	(segid 3A4 and resid 399 and name CA)	13.77	1.29	1.29
10	assign (segid 3A4 and resid 134 and name CA)	(segid 3A4 and resid 399 and name CB)	13.13	1.27	1.28
	assign (segid 3A4 and resid 134 and name CA)	(segid 3A4 and resid 400 and name CA)	11.59	1.18	1.17
	assign (segid 3A4 and resid 134 and name CA)	(segid 3A4 and resid 400 and name CB)	10.36	1.26	1.26
	assign (segid 3A4 and resid 134 and name CA)	(segid 3A4 and resid 401 and name CA)	14.55	1.21	1.20
	assign (segid 3A4 and resid 134 and name CA)	(segid 3A4 and resid 402 and name CA)	17.11	1.16	1.17
15	assign (segid 3A4 and resid 134 and name CA)	(segid 3A4 and resid 402 and name CB)	17.52	1.25	1.25
	assign (segid 3A4 and resid 134 and name CA)	(segid 3A4 and resid 403 and name CA)	15.80	0.93	0.93
	assign (segid 3A4 and resid 134 and name CA)	(segid 3A4 and resid 403 and name CB)	14.62	0.92	0.92
	assign (segid 3A4 and resid 134 and name CA)	(segid 3A4 and resid 404 and name CA)	15.42	0.72	0.71
	assign (segid 3A4 and resid 134 and name CA)	(segid 3A4 and resid 404 and name CB)	14.58	0.68	0.68
20	assign (segid 3A4 and resid 134 and name CA)	(segid 3A4 and resid 407 and name CB)	18.43	0.65	0.64
	assign (segid 3A4 and resid 134 and name N)	(segid 3A4 and resid 134 and name CA)	2.45	0.04	0.03
	assign (segid 3A4 and resid 134 and name N)	(segid 3A4 and resid 134 and name O)	3.50	0.04	0.04
	assign (segid 3A4 and resid 134 and name N)	(segid 3A4 and resid 135 and name C)	4.71	0.04	0.05
25	assign (segid 3A4 and resid 134 and name N)	(segid 3A4 and resid 135 and name CA)	4.21	0.06	0.06
	assign (segid 3A4 and resid 134 and name N)	(segid 3A4 and resid 135 and name CB)	4.98	0.08	0.07
	assign (segid 3A4 and resid 134 and name N)	(segid 3A4 and resid 135 and name N)	2.79	0.05	0.05
	assign (segid 3A4 and resid 134 and name N)	(segid 3A4 and resid 135 and name O)	5.77	0.05	0.05
	assign (segid 3A4 and resid 134 and name N)	(segid 3A4 and resid 136 and name C)	5.61	0.07	0.06
30	assign (segid 3A4 and resid 134 and name N)	(segid 3A4 and resid 136 and name CA)	5.38	0.12	0.11
	assign (segid 3A4 and resid 134 and name N)	(segid 3A4 and resid 136 and name CB)	5.52	0.29	0.28
	assign (segid 3A4 and resid 134 and name N)	(segid 3A4 and resid 136 and name N)	4.36	0.11	0.11
	assign (segid 3A4 and resid 134 and name N)	(segid 3A4 and resid 136 and name O)	6.79	0.05	0.06
	assign (segid 3A4 and resid 134 and name N)	(segid 3A4 and resid 137 and name C)	6.34	0.14	0.14
35	assign (segid 3A4 and resid 134 and name N)	(segid 3A4 and resid 137 and name CA)	5.51	0.15	0.14
	assign (segid 3A4 and resid 134 and name N)	(segid 3A4 and resid 137 and name N)	4.76	0.08	0.08
	assign (segid 3A4 and resid 134 and name N)	(segid 3A4 and resid 137 and name O)	7.52	0.14	0.14
	assign (segid 3A4 and resid 134 and name N)	(segid 3A4 and resid 138 and name CA)	7.07	0.15	0.15
	assign (segid 3A4 and resid 134 and name N)	(segid 3A4 and resid 138 and name CB)	6.89	0.19	0.18
40	assign (segid 3A4 and resid 134 and name N)	(segid 3A4 and resid 138 and name N)	5.97	0.14	0.14
	assign (segid 3A4 and resid 134 and name N)	(segid 3A4 and resid 135 and name C)	2.97	0.08	0.08
	assign (segid 3A4 and resid 134 and name O)	(segid 3A4 and resid 135 and name CA)	2.75	0.04	0.03
	assign (segid 3A4 and resid 134 and name O)	(segid 3A4 and resid 135 and name CB)	4.23	0.04	0.03
	assign (segid 3A4 and resid 134 and name O)	(segid 3A4 and resid 135 and name N)	2.24	0.02	0.02
45	assign (segid 3A4 and resid 134 and name O)	(segid 3A4 and resid 135 and name O)	3.40	0.11	0.11
	assign (segid 3A4 and resid 134 and name O)	(segid 3A4 and resid 136 and name C)	4.11	0.20	0.19
	assign (segid 3A4 and resid 134 and name O)	(segid 3A4 and resid 136 and name CA)	4.39	0.18	0.18
	assign (segid 3A4 and resid 134 and name O)	(segid 3A4 and resid 136 and name CB)	5.43	0.28	0.28
	assign (segid 3A4 and resid 134 and name O)	(segid 3A4 and resid 136 and name N)	3.46	0.18	0.17
50	assign (segid 3A4 and resid 134 and name O)	(segid 3A4 and resid 136 and name O)	5.06	0.22	0.23
	assign (segid 3A4 and resid 134 and name O)	(segid 3A4 and resid 137 and name C)	3.78	0.05	0.05
	assign (segid 3A4 and resid 134 and name O)	(segid 3A4 and resid 137 and name CA)	3.77	0.12	0.12
	assign (segid 3A4 and resid 134 and name O)	(segid 3A4 and resid 137 and name N)	3.26	0.17	0.17
	assign (segid 3A4 and resid 134 and name O)	(segid 3A4 and resid 137 and name O)	4.95	0.05	0.05
55	assign (segid 3A4 and resid 134 and name O)	(segid 3A4 and resid 138 and name C)	4.51	0.39	0.39
	assign (segid 3A4 and resid 134 and name O)	(segid 3A4 and resid 138 and name CA)	3.74	0.07	0.08
	assign (segid 3A4 and resid 134 and name O)	(segid 3A4 and resid 138 and name CB)	3.60	0.31	0.32
	assign (segid 3A4 and resid 134 and name O)	(segid 3A4 and resid 138 and name N)	2.91	0.04	0.05
	assign (segid 3A4 and resid 134 and name O)	(segid 3A4 and resid 138 and name O)	5.56	0.44	0.44
60	assign (segid 3A4 and resid 134 and name O)	(segid 3A4 and resid 139 and name C)	5.81	0.85	0.86
	assign (segid 3A4 and resid 134 and name O)	(segid 3A4 and resid 139 and name CA)	5.49	0.77	0.77
	assign (segid 3A4 and resid 134 and name O)	(segid 3A4 and resid 139 and name N)	4.35	0.58	0.59
	assign (segid 3A4 and resid 134 and name O)	(segid 3A4 and resid 140 and name C)	6.28	1.11	1.11
	assign (segid 3A4 and resid 134 and name O)	(segid 3A4 and resid 140 and name CA)	5.92	0.82	0.82
65	assign (segid 3A4 and resid 134 and name O)	(segid 3A4 and resid 140 and name CB)	5.70	0.58	0.59
	assign (segid 3A4 and resid 134 and name O)	(segid 3A4 and resid 140 and name N)	5.12	0.84	0.83
	assign (segid 3A4 and resid 134 and name O)	(segid 3A4 and resid 140 and name O)	5.62	1.28	1.29
	assign (segid 3A4 and resid 134 and name O)	(segid 3A4 and resid 219 and name CB)	7.28	0.58	0.58
	assign (segid 3A4 and resid 134 and name O)	(segid 3A4 and resid 220 and name N)	7.52	0.15	0.14
70	assign (segid 3A4 and resid 135 and name C)	(segid 3A4 and resid 135 and name CB)	2.52	0.03	0.02
	assign (segid 3A4 and resid 135 and name C)	(segid 3A4 and resid 135 and name O)	1.23	0.00	0.01
	assign (segid 3A4 and resid 135 and name C)	(segid 3A4 and resid 136 and name C)	3.09	0.06	0.05
	assign (segid 3A4 and resid 135 and name C)	(segid 3A4 and resid 136 and name CA)	2.44	0.01	0.01
	assign (segid 3A4 and resid 135 and name C)	(segid 3A4 and resid 136 and name CB)	3.72	0.02	0.02
75	assign (segid 3A4 and resid 135 and name C)	(segid 3A4 and resid 136 and name N)	1.33	0.00	0.00
	assign (segid 3A4 and resid 135 and name C)	(segid 3A4 and resid 136 and name O)	4.01	0.12	0.12
	assign (segid 3A4 and resid 135 and name C)	(segid 3A4 and resid 137 and name C)	4.69	0.10	0.10
	assign (segid 3A4 and resid 135 and name C)	(segid 3A4 and resid 137 and name CA)	4.53	0.05	0.05
	assign (segid 3A4 and resid 135 and name C)	(segid 3A4 and resid 137 and name N)	3.30	0.05	0.05
80	assign (segid 3A4 and resid 135 and name C)	(segid 3A4 and resid 137 and name O)	5.75	0.14	0.15
	assign (segid 3A4 and resid 135 and name C)	(segid 3A4 and resid 138 and name C)	4.85	0.12	0.13
	assign (segid 3A4 and resid 135 and name C)	(segid 3A4 and resid 138 and name CA)	4.81	0.28	0.29

	assign (segid 3A4 and resid 135 and name C) (segid 3A4 and resid 138 and name CB)	5.05	0.68	0.68
	assign (segid 3A4 and resid 135 and name C) (segid 3A4 and resid 138 and name N)	4.03	0.20	0.20
	assign (segid 3A4 and resid 135 and name C) (segid 3A4 and resid 138 and name O)	5.93	0.14	0.15
	assign (segid 3A4 and resid 135 and name C) (segid 3A4 and resid 139 and name C)	4.83	0.12	0.11
5	assign (segid 3A4 and resid 135 and name C) (segid 3A4 and resid 139 and name CA)	4.57	0.29	0.29
	assign (segid 3A4 and resid 135 and name C) (segid 3A4 and resid 139 and name N)	4.00	0.07	0.06
	assign (segid 3A4 and resid 135 and name C) (segid 3A4 and resid 139 and name O)	5.85	0.27	0.28
	assign (segid 3A4 and resid 135 and name C) (segid 3A4 and resid 140 and name C)	5.14	0.38	0.38
	assign (segid 3A4 and resid 135 and name C) (segid 3A4 and resid 140 and name CA)	5.10	0.51	0.51
	assign (segid 3A4 and resid 135 and name C) (segid 3A4 and resid 140 and name CB)	5.31	0.98	0.97
10	assign (segid 3A4 and resid 135 and name C) (segid 3A4 and resid 140 and name N)	4.31	0.36	0.35
	assign (segid 3A4 and resid 135 and name C) (segid 3A4 and resid 140 and name O)	4.38	0.40	0.39
	assign (segid 3A4 and resid 135 and name C) (segid 3A4 and resid 141 and name CA)	6.94	0.26	0.26
	assign (segid 3A4 and resid 135 and name C) (segid 3A4 and resid 141 and name N)	6.35	0.31	0.31
	assign (segid 3A4 and resid 135 and name C) (segid 3A4 and resid 141 and name O)	6.75	0.86	0.86
15	assign (segid 3A4 and resid 135 and name C) (segid 3A4 and resid 141 and name CB)	1.52	0.01	0.00
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 135 and name C)	1.52	0.01	0.02
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 135 and name O)	2.38	0.01	0.02
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 136 and name C)	4.45	0.05	0.06
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 136 and name CA)	3.82	0.02	0.01
20	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 136 and name CB)	4.89	0.06	0.05
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 136 and name N)	2.45	0.02	0.02
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 136 and name O)	5.45	0.13	0.12
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 137 and name C)	5.58	0.07	0.07
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 137 and name CA)	5.48	0.07	0.07
25	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 137 and name N)	4.36	0.05	0.04
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 137 and name O)	6.71	0.10	0.09
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 138 and name C)	5.47	0.15	0.15
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 138 and name CA)	5.32	0.20	0.21
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 138 and name CB)	5.17	0.67	0.67
30	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 138 and name N)	4.70	0.11	0.12
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 138 and name O)	6.46	0.26	0.26
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 139 and name C)	5.28	0.55	0.55
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 139 and name CA)	5.34	0.68	0.67
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 139 and name N)	4.77	0.36	0.36
35	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 139 and name O)	6.25	0.71	0.71
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 140 and name C)	4.99	0.46	0.46
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 140 and name CA)	5.00	0.22	0.21
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 140 and name CB)	4.93	0.70	0.69
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 140 and name N)	4.52	0.26	0.26
40	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 140 and name O)	4.25	0.63	0.63
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 141 and name CA)	6.70	0.77	0.76
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 141 and name CB)	7.76	1.10	1.10
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 141 and name N)	6.13	0.55	0.54
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 141 and name O)	7.16	0.48	0.47
45	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 141 and name CB)	10.84	3.49	3.49
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 147 and name CA)	11.80	3.56	3.56
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 148 and name CA)	11.95	1.62	1.63
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 149 and name CA)	10.46	1.54	1.53
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 149 and name CB)	9.92	1.48	1.48
50	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 150 and name CA)	10.60	3.38	3.39
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 151 and name CA)	13.20	2.59	2.58
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 152 and name CA)	12.99	1.48	1.48
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 152 and name CB)	12.65	0.97	0.97
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 153 and name CA)	11.83	2.87	2.87
55	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 153 and name CB)	10.92	3.30	3.29
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 156 and name CB)	14.50	2.33	2.33
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 193 and name CA)	17.48	1.21	1.21
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 193 and name CB)	17.55	1.25	1.25
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 194 and name CA)	14.37	1.36	1.35
60	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 194 and name CB)	14.18	1.53	1.53
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 195 and name CA)	16.00	1.21	1.20
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 195 and name CB)	17.36	1.25	1.25
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 196 and name CA)	16.83	0.87	0.87
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 196 and name CB)	17.70	0.88	0.88
65	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 197 and name CA)	13.47	0.74	0.74
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 197 and name CB)	12.67	0.82	0.81
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 198 and name CA)	12.22	0.75	0.74
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 198 and name CB)	12.27	0.85	0.84
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 199 and name CA)	15.51	0.66	0.65
70	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 199 and name CB)	16.82	0.69	0.69
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 200 and name CA)	15.28	0.63	0.64
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 201 and name CA)	12.11	0.63	0.62
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 201 and name CB)	10.73	0.56	0.56
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 202 and name CA)	13.96	0.54	0.55
75	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 202 and name CB)	14.58	0.50	0.50
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 203 and name CA)	17.03	0.62	0.62
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 203 and name CB)	17.79	0.59	0.58
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 204 and name CA)	15.68	0.63	0.64
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 204 and name CB)	14.75	0.56	0.56
80	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 205 and name CA)	14.26	0.74	0.73
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 205 and name CB)	13.15	0.65	0.65
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 206 and name CA)	17.70	0.67	0.66

	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 206 and name CB)	18.45	0.59	0.59
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 219 and name CA)	8.94	0.80	0.80
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 219 and name CB)	7.97	0.84	0.84
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 220 and name CA)	9.68	0.22	0.22
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 220 and name CB)	9.10	0.17	0.17
5	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 221 and name CA)	10.48	0.23	0.23
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 221 and name CB)	9.80	0.29	0.30
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 222 and name CA)	12.82	0.38	0.37
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 222 and name CB)	12.71	0.49	0.49
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 223 and name CA)	14.35	0.34	0.33
10	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 223 and name CB)	13.89	0.32	0.32
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 224 and name CA)	15.04	0.15	0.16
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 224 and name CB)	14.24	0.19	0.19
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 225 and name CA)	16.41	0.24	0.24
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 225 and name CB)	15.82	0.22	0.22
15	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 226 and name CA)	18.72	0.34	0.34
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 244 and name CA)	16.08	0.62	0.62
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 244 and name CB)	16.10	0.60	0.60
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 245 and name CA)	15.05	0.79	0.79
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 245 and name CB)	16.01	0.84	0.84
20	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 246 and name CA)	16.27	0.89	0.88
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 246 and name CB)	17.72	0.89	0.89
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 247 and name CA)	14.44	0.72	0.71
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 247 and name CB)	14.66	0.58	0.58
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 248 and name CA)	11.03	0.76	0.76
25	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 248 and name CB)	10.81	0.74	0.75
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 249 and name CA)	12.26	1.10	1.10
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 250 and name CA)	13.51	0.99	0.98
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 250 and name CB)	14.57	0.93	0.93
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 251 and name CA)	10.58	0.82	0.82
30	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 251 and name CB)	9.94	0.65	0.65
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 252 and name CA)	8.81	1.31	1.30
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 252 and name CB)	8.73	1.38	1.39
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 253 and name CA)	12.12	1.48	1.48
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 254 and name CA)	13.37	1.28	1.27
35	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 255 and name CA)	10.88	1.44	1.43
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 256 and name CA)	10.52	1.12	1.12
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 257 and name CA)	14.10	1.20	1.20
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 258 and name CA)	15.74	1.01	1.01
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 258 and name CB)	15.81	0.96	0.96
40	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 259 and name CA)	14.15	0.64	0.65
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 259 and name CB)	12.86	0.59	0.59
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 260 and name CA)	14.64	0.76	0.75
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 260 and name CB)	14.22	0.81	0.81
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 261 and name CA)	18.17	0.80	0.81
45	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 262 and name CA)	18.91	0.56	0.56
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 262 and name CB)	18.32	0.53	0.53
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 263 and name CA)	18.16	0.39	0.40
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 263 and name CB)	16.89	0.36	0.36
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 391 and name CA)	18.87	0.57	0.56
50	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 391 and name CB)	18.51	0.56	0.57
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 392 and name CA)	16.89	0.60	0.60
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 392 and name CB)	16.41	0.66	0.65
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 393 and name CA)	14.21	0.48	0.49
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 394 and name CA)	17.08	0.42	0.42
55	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 394 and name CB)	18.50	0.42	0.43
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 395 and name CA)	16.60	0.49	0.49
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 396 and name CA)	13.00	0.44	0.44
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 396 and name CB)	11.79	0.49	0.48
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 397 and name CA)	14.17	0.38	0.38
60	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 397 and name CB)	14.91	0.38	0.38
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 398 and name CA)	17.22	0.43	0.43
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 398 and name CB)	18.34	0.48	0.47
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 399 and name CA)	15.67	0.59	0.59
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 399 and name CB)	14.92	0.69	0.70
65	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 400 and name CA)	13.48	0.54	0.53
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 400 and name CB)	12.40	0.49	0.49
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 401 and name CA)	16.62	0.56	0.56
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 402 and name CA)	18.91	0.64	0.64
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 403 and name CA)	17.09	0.77	0.78
70	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 403 and name CB)	15.81	0.78	0.78
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 404 and name CA)	16.74	0.87	0.88
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 404 and name CB)	16.05	0.88	0.87
	assign (segid 3A4 and resid 135 and name CA) (segid 3A4 and resid 136 and name C)	5.51	0.06	0.07
	assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 136 and name CA)	4.54	0.08	0.08
75	assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 136 and name CB)	5.41	0.08	0.07
	assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 136 and name N)	3.21	0.09	0.09
	assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 136 and name O)	6.47	0.12	0.12
	assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 137 and name C)	7.02	0.08	0.07
	assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 137 and name CA)	6.86	0.07	0.07
80	assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 137 and name N)	5.63	0.06	0.06
	assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 138 and name C)	6.67	0.13	0.13
	assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 138 and name CA)	6.70	0.26	0.26

	assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 138 and name CB)	6.51	0.76	0.75
	assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 138 and name N)	6.16	0.14	0.15
	assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 139 and name C)	5.83	0.44	0.45
	assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 139 and name CA)	6.14	0.61	0.61
	assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 139 and name N)	5.86	0.27	0.26
5	assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 139 and name O)	6.61	0.66	0.67
	assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 140 and name C)	4.88	0.42	0.41
	assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 140 and name CA)	5.18	0.36	0.36
	assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 140 and name CB)	5.11	1.06	1.06
	assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 140 and name N)	5.04	0.21	0.21
10	assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 140 and name O)	4.13	0.61	0.60
	assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 141 and name C)	6.33	0.63	0.63
	assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 141 and name CA)	6.17	0.67	0.67
	assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 141 and name CB)	7.12	1.03	1.04
	assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 141 and name N)	5.82	0.45	0.44
15	assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 141 and name O)	6.44	0.87	0.88
	assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 147 and name CA)	10.16	4.13	4.13
	assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 147 and name CB)	11.16	4.20	4.20
	assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 148 and name CA)	11.33	2.37	2.37
	assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 149 and name CA)	9.84	2.17	2.17
20	assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 149 and name CB)	9.37	1.99	1.99
	assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 150 and name CA)	9.84	4.05	4.04
	assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 151 and name CA)	12.56	3.35	3.34
	assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 152 and name CA)	12.52	2.16	2.15
	assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 152 and name CB)	12.20	1.53	1.53
25	assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 153 and name CA)	11.45	3.38	3.38
	assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 153 and name CB)	10.53	3.76	3.76
	assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 193 and name CB)	17.57	1.69	1.69
	assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 194 and name CA)	14.63	1.78	1.79
	assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 194 and name CB)	14.48	1.97	1.97
30	assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 195 and name CA)	16.51	1.56	1.57
	assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 196 and name CA)	17.19	1.24	1.23
	assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 196 and name CB)	17.97	1.28	1.27
	assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 197 and name CA)	13.73	1.14	1.15
	assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 197 and name CB)	12.85	1.25	1.26
35	assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 198 and name CA)	12.84	1.00	1.00
	assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 198 and name CB)	12.97	1.09	1.10
	assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 199 and name CA)	16.18	0.85	0.84
	assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 199 and name CB)	17.45	0.92	0.92
40	assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 200 and name CA)	15.78	0.84	0.84
	assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 201 and name CA)	12.74	0.73	0.72
	assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 201 and name CB)	11.39	0.67	0.66
	assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 202 and name CA)	14.86	0.57	0.57
	assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 202 and name CB)	15.51	0.55	0.55
45	assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 203 and name CA)	17.79	0.67	0.66
	assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 203 and name CB)	18.47	0.68	0.68
	assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 204 and name CA)	16.31	0.67	0.67
	assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 204 and name CB)	15.29	0.67	0.67
	assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 205 and name CA)	15.10	0.67	0.68
50	assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 205 and name CB)	14.08	0.61	0.60
	assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 206 and name CA)	18.61	0.61	0.61
	assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 206 and name CB)	10.04	0.91	0.90
	assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 219 and name CB)	9.04	0.86	0.87
	assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 220 and name CA)	10.99	0.31	0.31
55	assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 220 and name CB)	10.46	0.23	0.23
	assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 221 and name CA)	11.71	0.25	0.24
	assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 221 and name CB)	10.97	0.39	0.38
	assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 222 and name CA)	13.93	0.34	0.34
	assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 222 and name CB)	13.76	0.49	0.49
60	assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 223 and name CA)	15.57	0.42	0.42
	assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 223 and name CB)	15.14	0.46	0.45
	assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 224 and name CA)	16.32	0.13	0.14
	assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 224 and name CB)	15.54	0.21	0.20
	assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 225 and name CA)	17.57	0.25	0.26
	assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 225 and name CB)	16.93	0.24	0.24
65	assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 244 and name CA)	17.24	0.60	0.61
	assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 244 and name CB)	17.26	0.56	0.56
	assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 245 and name CA)	16.05	0.85	0.85
	assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 245 and name CB)	16.93	0.94	0.94
	assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 246 and name CA)	17.26	0.95	0.96
70	assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 247 and name CA)	15.59	0.69	0.68
	assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 247 and name CB)	15.87	0.53	0.53
	assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 248 and name CA)	12.15	0.77	0.76
	assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 248 and name CB)	11.90	0.78	0.77
	assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 249 and name CA)	13.11	1.22	1.22
75	assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 250 and name CA)	14.44	1.03	1.02
	assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 250 and name CB)	15.56	0.93	0.94
	assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 251 and name CA)	11.62	0.74	0.75
	assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 251 and name CB)	11.09	0.55	0.54
	assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 252 and name CA)	9.56	1.34	1.34
80	assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 252 and name CB)	9.42	1.49	1.49
	assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 253 and name CA)	12.65	1.59	1.60
	assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 254 and name CA)	14.05	1.24	1.24

assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 255 and name CA) 11.49 1.33 1.33
 assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 256 and name CA) 10.73 1.13 1.14
 assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 257 and name CA) 14.19 1.24 1.23
 assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 258 and name CA) 15.97 0.92 0.93
 assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 258 and name CB) 16.17 0.86 0.85
 5 assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 259 and name CA) 14.28 0.48 0.49
 assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 259 and name CB) 13.03 0.45 0.44
 assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 260 and name CA) 14.45 0.69 0.68
 assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 260 and name CB) 13.98 0.79 0.79
 assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 261 and name CA) 18.05 0.74 0.74
 10 assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 262 and name CA) 18.88 0.38 0.38
 assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 262 and name CB) 18.38 0.32 0.32
 assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 263 and name CA) 17.93 0.24 0.24
 assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 263 and name CB) 16.60 0.23 0.23
 assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 392 and name CA) 17.93 0.64 0.65
 15 assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 392 and name CB) 17.51 0.66 0.67
 assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 393 and name CA) 15.13 0.59 0.59
 assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 393 and name CB) 17.82 0.59 0.59
 assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 394 and name CA) 19.27 0.61 0.61
 assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 394 and name CB) 17.32 0.91 0.90
 20 assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 395 and name CA) 13.65 0.87 0.87
 assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 396 and name CA) 12.52 0.89 0.89
 assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 396 and name CB) 14.63 0.64 0.65
 assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 397 and name CA) 15.41 0.56 0.56
 assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 397 and name CB) 17.59 0.83 0.83
 25 assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 398 and name CA) 18.76 0.90 0.90
 assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 398 and name CB) 15.96 1.12 1.12
 assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 399 and name CA) 15.28 1.25 1.24
 assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 399 and name CB) 13.56 0.95 0.96
 assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 400 and name CA) 12.53 0.79 0.79
 30 assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 400 and name CB) 16.62 0.85 0.85
 assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 401 and name CA) 16.93 1.30 1.29
 assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 401 and name CB) 15.67 1.33 1.32
 assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 402 and name CA) 16.39 1.29 1.30
 assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 402 and name CB) 15.71 1.24 1.25
 35 assign (segid 3A4 and resid 135 and name CB) (segid 3A4 and resid 403 and name CA) 2.44 0.02 0.03
 assign (segid 3A4 and resid 135 and name N) (segid 3A4 and resid 135 and name C) 1.46 0.01 0.01
 assign (segid 3A4 and resid 135 and name N) (segid 3A4 and resid 135 and name CB) 2.46 0.02 0.01
 assign (segid 3A4 and resid 135 and name N) (segid 3A4 and resid 135 and name O) 3.47 0.04 0.05
 assign (segid 3A4 and resid 135 and name N) (segid 3A4 and resid 136 and name C) 4.69 0.09 0.09
 40 assign (segid 3A4 and resid 135 and name N) (segid 3A4 and resid 136 and name CA) 4.21 0.07 0.06
 assign (segid 3A4 and resid 135 and name N) (segid 3A4 and resid 136 and name CB) 5.00 0.16 0.16
 assign (segid 3A4 and resid 135 and name N) (segid 3A4 and resid 136 and name N) 2.81 0.07 0.07
 assign (segid 3A4 and resid 135 and name N) (segid 3A4 and resid 136 and name O) 5.82 0.12 0.12
 assign (segid 3A4 and resid 135 and name N) (segid 3A4 and resid 137 and name C) 5.61 0.07 0.07
 45 assign (segid 3A4 and resid 135 and name N) (segid 3A4 and resid 137 and name CA) 5.27 0.10 0.10
 assign (segid 3A4 and resid 135 and name N) (segid 3A4 and resid 137 and name N) 4.24 0.06 0.06
 assign (segid 3A4 and resid 135 and name N) (segid 3A4 and resid 137 and name O) 6.81 0.08 0.07
 assign (segid 3A4 and resid 135 and name N) (segid 3A4 and resid 138 and name C) 6.10 0.26 0.26
 50 assign (segid 3A4 and resid 135 and name N) (segid 3A4 and resid 138 and name CA) 5.64 0.08 0.09
 assign (segid 3A4 and resid 135 and name N) (segid 3A4 and resid 138 and name CB) 5.42 0.47 0.47
 assign (segid 3A4 and resid 135 and name N) (segid 3A4 and resid 138 and name N) 4.83 0.03 0.04
 assign (segid 3A4 and resid 135 and name N) (segid 3A4 and resid 138 and name O) 7.15 0.34 0.33
 assign (segid 3A4 and resid 135 and name N) (segid 3A4 and resid 139 and name C) 6.39 0.71 0.72
 55 assign (segid 3A4 and resid 135 and name N) (segid 3A4 and resid 139 and name CA) 6.37 0.72 0.72
 assign (segid 3A4 and resid 135 and name N) (segid 3A4 and resid 139 and name N) 5.58 0.45 0.46
 assign (segid 3A4 and resid 135 and name N) (segid 3A4 and resid 140 and name C) 5.97 0.85 0.85
 assign (segid 3A4 and resid 135 and name N) (segid 3A4 and resid 140 and name CB) 6.03 0.46 0.47
 assign (segid 3A4 and resid 135 and name N) (segid 3A4 and resid 140 and name N) 5.83 0.34 0.34
 60 assign (segid 3A4 and resid 135 and name N) (segid 3A4 and resid 140 and name O) 5.57 0.54 0.53
 assign (segid 3A4 and resid 135 and name N) (segid 3A4 and resid 140 and name N) 5.13 1.05 1.04
 assign (segid 3A4 and resid 135 and name N) (segid 3A4 and resid 140 and name CB) 3.31 0.05 0.05
 assign (segid 3A4 and resid 135 and name O) (segid 3A4 and resid 135 and name CB) 3.05 0.08 0.08
 assign (segid 3A4 and resid 135 and name O) (segid 3A4 and resid 136 and name C) 2.74 0.02 0.03
 assign (segid 3A4 and resid 135 and name O) (segid 3A4 and resid 136 and name CA) 4.23 0.03 0.03
 65 assign (segid 3A4 and resid 135 and name O) (segid 3A4 and resid 136 and name CB) 2.23 0.00 0.01
 assign (segid 3A4 and resid 135 and name O) (segid 3A4 and resid 136 and name N) 3.66 0.20 0.19
 assign (segid 3A4 and resid 135 and name O) (segid 3A4 and resid 136 and name O) 4.31 0.19 0.19
 assign (segid 3A4 and resid 135 and name O) (segid 3A4 and resid 137 and name C) 4.48 0.10 0.11
 assign (segid 3A4 and resid 135 and name O) (segid 3A4 and resid 137 and name CA) 3.46 0.08 0.08
 70 assign (segid 3A4 and resid 135 and name O) (segid 3A4 and resid 137 and name N) 5.23 0.24 0.23
 assign (segid 3A4 and resid 135 and name O) (segid 3A4 and resid 137 and name O) 3.93 0.24 0.24
 assign (segid 3A4 and resid 135 and name O) (segid 3A4 and resid 138 and name C) 4.14 0.39 0.39
 assign (segid 3A4 and resid 135 and name O) (segid 3A4 and resid 138 and name CB) 4.53 0.79 0.79
 assign (segid 3A4 and resid 135 and name O) (segid 3A4 and resid 138 and name N) 3.59 0.28 0.28
 75 assign (segid 3A4 and resid 135 and name O) (segid 3A4 and resid 138 and name O) 4.96 0.22 0.22
 assign (segid 3A4 and resid 135 and name O) (segid 3A4 and resid 139 and name C) 3.86 0.23 0.23
 assign (segid 3A4 and resid 135 and name O) (segid 3A4 and resid 139 and name CA) 3.48 0.19 0.20
 assign (segid 3A4 and resid 135 and name O) (segid 3A4 and resid 139 and name N) 2.98 0.10 0.11
 80 assign (segid 3A4 and resid 135 and name O) (segid 3A4 and resid 139 and name O) 4.90 0.24 0.24
 assign (segid 3A4 and resid 135 and name O) (segid 3A4 and resid 140 and name C) 4.79 0.65 0.65
 assign (segid 3A4 and resid 135 and name O) (segid 3A4 and resid 140 and name CA) 4.52 0.75 0.74
 assign (segid 3A4 and resid 135 and name O) (segid 3A4 and resid 140 and name CB) 4.91 1.10 1.10

	assign (segid 3A4 and resid 135 and name O)	(segid 3A4 and resid 140 and name N)	3.50	0.62	0.63
	assign (segid 3A4 and resid 135 and name O)	(segid 3A4 and resid 140 and name O)	4.22	0.63	0.64
	assign (segid 3A4 and resid 135 and name O)	(segid 3A4 and resid 141 and name CA)	6.79	0.49	0.49
	assign (segid 3A4 and resid 135 and name O)	(segid 3A4 and resid 141 and name N)	6.03	0.59	0.58
	assign (segid 3A4 and resid 135 and name O)	(segid 3A4 and resid 219 and name CA)	6.79	0.89	0.90
5	assign (segid 3A4 and resid 135 and name O)	(segid 3A4 and resid 219 and name CB)	5.77	0.88	0.87
	assign (segid 3A4 and resid 135 and name O)	(segid 3A4 and resid 219 and name CG)	6.54	0.80	0.80
	assign (segid 3A4 and resid 135 and name O)	(segid 3A4 and resid 220 and name N)	7.11	0.51	0.50
	assign (segid 3A4 and resid 136 and name C)	(segid 3A4 and resid 136 and name CB)	2.49	0.03	0.03
	assign (segid 3A4 and resid 136 and name C)	(segid 3A4 and resid 136 and name O)	1.22	0.00	0.01
10	assign (segid 3A4 and resid 136 and name C)	(segid 3A4 and resid 137 and name C)	3.11	0.17	0.17
	assign (segid 3A4 and resid 136 and name C)	(segid 3A4 and resid 137 and name CA)	2.42	0.01	0.02
	assign (segid 3A4 and resid 136 and name C)	(segid 3A4 and resid 137 and name N)	1.33	0.01	0.01
	assign (segid 3A4 and resid 136 and name C)	(segid 3A4 and resid 137 and name O)	3.94	0.21	0.20
	assign (segid 3A4 and resid 136 and name C)	(segid 3A4 and resid 138 and name C)	4.90	0.36	0.36
15	assign (segid 3A4 and resid 136 and name C)	(segid 3A4 and resid 138 and name CA)	4.66	0.28	0.28
	assign (segid 3A4 and resid 136 and name C)	(segid 3A4 and resid 138 and name CB)	5.57	0.37	0.37
	assign (segid 3A4 and resid 136 and name C)	(segid 3A4 and resid 138 and name N)	3.44	0.25	0.24
	assign (segid 3A4 and resid 136 and name C)	(segid 3A4 and resid 138 and name O)	6.04	0.36	0.35
	assign (segid 3A4 and resid 136 and name C)	(segid 3A4 and resid 139 and name C)	5.89	0.55	0.56
20	assign (segid 3A4 and resid 136 and name C)	(segid 3A4 and resid 139 and name CA)	4.97	0.42	0.42
	assign (segid 3A4 and resid 136 and name C)	(segid 3A4 and resid 139 and name N)	4.18	0.43	0.42
	assign (segid 3A4 and resid 136 and name C)	(segid 3A4 and resid 139 and name O)	6.94	0.52	0.52
	assign (segid 3A4 and resid 136 and name C)	(segid 3A4 and resid 140 and name N)	5.86	0.68	0.67
	assign (segid 3A4 and resid 136 and name C)	(segid 3A4 and resid 140 and name O)	6.38	0.70	0.70
25	assign (segid 3A4 and resid 136 and name C)	(segid 3A4 and resid 219 and name C)	6.31	0.90	0.91
	assign (segid 3A4 and resid 136 and name C)	(segid 3A4 and resid 219 and name CA)	5.67	0.77	0.77
	assign (segid 3A4 and resid 136 and name C)	(segid 3A4 and resid 219 and name CB)	5.13	0.73	0.73
	assign (segid 3A4 and resid 136 and name C)	(segid 3A4 and resid 219 and name CG)	6.30	0.77	0.78
	assign (segid 3A4 and resid 136 and name C)	(segid 3A4 and resid 219 and name N)	6.84	0.70	0.69
30	assign (segid 3A4 and resid 136 and name C)	(segid 3A4 and resid 220 and name CA)	6.79	0.99	0.98
	assign (segid 3A4 and resid 136 and name C)	(segid 3A4 and resid 220 and name CB)	6.44	1.00	1.00
	assign (segid 3A4 and resid 136 and name C)	(segid 3A4 and resid 220 and name N)	5.77	0.95	0.96
	assign (segid 3A4 and resid 136 and name CA)	(segid 3A4 and resid 136 and name C)	1.53	0.01	0.00
	assign (segid 3A4 and resid 136 and name CA)	(segid 3A4 and resid 136 and name CB)	1.54	0.02	0.02
35	assign (segid 3A4 and resid 136 and name CA)	(segid 3A4 and resid 136 and name O)	2.39	0.02	0.02
	assign (segid 3A4 and resid 136 and name CA)	(segid 3A4 and resid 137 and name C)	4.49	0.13	0.13
	assign (segid 3A4 and resid 136 and name CA)	(segid 3A4 and resid 137 and name CA)	3.81	0.01	0.01
	assign (segid 3A4 and resid 136 and name CA)	(segid 3A4 and resid 137 and name N)	2.44	0.03	0.04
40	assign (segid 3A4 and resid 136 and name CA)	(segid 3A4 and resid 137 and name O)	5.39	0.19	0.18
	assign (segid 3A4 and resid 136 and name CA)	(segid 3A4 and resid 138 and name C)	5.72	0.30	0.30
	assign (segid 3A4 and resid 136 and name CA)	(segid 3A4 and resid 138 and name CB)	5.65	0.27	0.27
	assign (segid 3A4 and resid 136 and name CA)	(segid 3A4 and resid 138 and name N)	6.35	0.47	0.48
	assign (segid 3A4 and resid 136 and name CA)	(segid 3A4 and resid 138 and name O)	4.52	0.22	0.22
45	assign (segid 3A4 and resid 136 and name CA)	(segid 3A4 and resid 139 and name C)	6.84	0.29	0.30
	assign (segid 3A4 and resid 136 and name CA)	(segid 3A4 and resid 139 and name CA)	5.96	0.53	0.52
	assign (segid 3A4 and resid 136 and name CA)	(segid 3A4 and resid 139 and name N)	5.31	0.29	0.28
	assign (segid 3A4 and resid 136 and name CA)	(segid 3A4 and resid 139 and name O)	4.78	0.33	0.32
	assign (segid 3A4 and resid 136 and name CA)	(segid 3A4 and resid 140 and name CA)	6.79	0.90	0.89
50	assign (segid 3A4 and resid 136 and name CA)	(segid 3A4 and resid 140 and name CB)	7.24	1.15	1.15
	assign (segid 3A4 and resid 136 and name CA)	(segid 3A4 and resid 140 and name N)	5.79	0.75	0.76
	assign (segid 3A4 and resid 136 and name CA)	(segid 3A4 and resid 140 and name O)	5.75	0.91	0.90
	assign (segid 3A4 and resid 136 and name CA)	(segid 3A4 and resid 141 and name CA)	8.21	0.80	0.80
	assign (segid 3A4 and resid 136 and name CA)	(segid 3A4 and resid 141 and name CB)	9.26	0.56	0.55
	assign (segid 3A4 and resid 136 and name CA)	(segid 3A4 and resid 148 and name CA)	13.63	2.22	2.21
55	assign (segid 3A4 and resid 136 and name CA)	(segid 3A4 and resid 149 and name CA)	12.78	1.78	1.78
	assign (segid 3A4 and resid 136 and name CA)	(segid 3A4 and resid 149 and name CB)	12.30	1.75	1.76
	assign (segid 3A4 and resid 136 and name CA)	(segid 3A4 and resid 150 and name CA)	13.17	3.48	3.49
	assign (segid 3A4 and resid 136 and name CA)	(segid 3A4 and resid 152 and name CA)	15.62	1.20	1.21
	assign (segid 3A4 and resid 136 and name CA)	(segid 3A4 and resid 152 and name CB)	15.22	0.89	0.90
60	assign (segid 3A4 and resid 136 and name CA)	(segid 3A4 and resid 153 and name CA)	14.71	2.30	2.29
	assign (segid 3A4 and resid 136 and name CA)	(segid 3A4 and resid 153 and name CB)	13.85	2.76	2.76
	assign (segid 3A4 and resid 136 and name CA)	(segid 3A4 and resid 194 and name CA)	16.97	1.09	1.08
	assign (segid 3A4 and resid 136 and name CA)	(segid 3A4 and resid 194 and name CB)	16.77	1.10	1.11
	assign (segid 3A4 and resid 136 and name CA)	(segid 3A4 and resid 195 and name CA)	18.19	1.02	1.03
65	assign (segid 3A4 and resid 136 and name CA)	(segid 3A4 and resid 197 and name CA)	15.78	0.82	0.82
	assign (segid 3A4 and resid 136 and name CA)	(segid 3A4 and resid 197 and name CB)	15.16	0.86	0.87
	assign (segid 3A4 and resid 136 and name CA)	(segid 3A4 and resid 198 and name CA)	14.06	0.90	0.91
	assign (segid 3A4 and resid 136 and name CA)	(segid 3A4 and resid 198 and name CB)	14.10	0.94	0.94
	assign (segid 3A4 and resid 136 and name CA)	(segid 3A4 and resid 199 and name CA)	17.00	0.93	0.92
70	assign (segid 3A4 and resid 136 and name CA)	(segid 3A4 and resid 200 and name CA)	16.73	0.74	0.74
	assign (segid 3A4 and resid 136 and name CA)	(segid 3A4 and resid 201 and name CA)	13.25	0.69	0.69
	assign (segid 3A4 and resid 136 and name CA)	(segid 3A4 and resid 201 and name CB)	12.02	0.68	0.69
	assign (segid 3A4 and resid 136 and name CA)	(segid 3A4 and resid 202 and name CA)	14.60	0.75	0.76
	assign (segid 3A4 and resid 136 and name CA)	(segid 3A4 and resid 202 and name CB)	15.30	0.80	0.81
75	assign (segid 3A4 and resid 136 and name CA)	(segid 3A4 and resid 203 and name CA)	17.62	0.71	0.71
	assign (segid 3A4 and resid 136 and name CA)	(segid 3A4 and resid 204 and name CA)	16.08	0.69	0.70
	assign (segid 3A4 and resid 136 and name CA)	(segid 3A4 and resid 204 and name CB)	15.31	0.72	0.72
	assign (segid 3A4 and resid 136 and name CA)	(segid 3A4 and resid 205 and name CA)	14.09	0.70	0.70
	assign (segid 3A4 and resid 136 and name CA)	(segid 3A4 and resid 205 and name CB)	12.99	0.65	0.65
80	assign (segid 3A4 and resid 136 and name CA)	(segid 3A4 and resid 206 and name CA)	17.41	0.71	0.70
	assign (segid 3A4 and resid 136 and name CA)	(segid 3A4 and resid 206 and name CB)	18.32	0.69	0.68
	assign (segid 3A4 and resid 136 and name CA)	(segid 3A4 and resid 219 and name CA)	6.81	1.01	1.00

5	assign	(segid 3A4 and resid 136 and name CA)	(segid 3A4 and resid 219 and name CB)	6.19	0.88	0.87
	assign	(segid 3A4 and resid 136 and name CA)	(segid 3A4 and resid 220 and name CA)	8.17	1.03	1.04
	assign	(segid 3A4 and resid 136 and name CA)	(segid 3A4 and resid 220 and name CB)	7.83	1.02	1.02
	assign	(segid 3A4 and resid 136 and name CA)	(segid 3A4 and resid 221 and name CA)	9.90	0.70	0.71
	assign	(segid 3A4 and resid 136 and name CA)	(segid 3A4 and resid 221 and name CB)	9.59	0.54	0.54
	assign	(segid 3A4 and resid 136 and name CA)	(segid 3A4 and resid 222 and name CA)	11.61	0.78	0.79
	assign	(segid 3A4 and resid 136 and name CA)	(segid 3A4 and resid 222 and name CB)	11.27	0.73	0.73
	assign	(segid 3A4 and resid 136 and name CA)	(segid 3A4 and resid 223 and name CA)	12.72	1.03	1.03
	assign	(segid 3A4 and resid 136 and name CA)	(segid 3A4 and resid 223 and name CB)	12.09	1.07	1.07
10	assign	(segid 3A4 and resid 136 and name CA)	(segid 3A4 and resid 224 and name CA)	14.13	0.95	0.94
	assign	(segid 3A4 and resid 136 and name CA)	(segid 3A4 and resid 224 and name CB)	13.60	0.89	0.89
	assign	(segid 3A4 and resid 136 and name CA)	(segid 3A4 and resid 225 and name CA)	15.75	0.78	0.77
	assign	(segid 3A4 and resid 136 and name CA)	(segid 3A4 and resid 225 and name CB)	15.22	0.69	0.69
	assign	(segid 3A4 and resid 136 and name CA)	(segid 3A4 and resid 226 and name CA)	17.50	0.92	0.91
15	assign	(segid 3A4 and resid 136 and name CA)	(segid 3A4 and resid 244 and name CA)	16.45	1.33	1.32
	assign	(segid 3A4 and resid 136 and name CA)	(segid 3A4 and resid 244 and name CB)	16.37	1.33	1.32
	assign	(segid 3A4 and resid 136 and name CA)	(segid 3A4 and resid 245 and name CA)	16.16	1.24	1.23
	assign	(segid 3A4 and resid 136 and name CA)	(segid 3A4 and resid 245 and name CB)	17.27	1.21	1.20
	assign	(segid 3A4 and resid 136 and name CA)	(segid 3A4 and resid 246 and name CA)	17.45	1.16	1.17
20	assign	(segid 3A4 and resid 136 and name CA)	(segid 3A4 and resid 247 and name CA)	15.09	1.31	1.32
	assign	(segid 3A4 and resid 136 and name CA)	(segid 3A4 and resid 247 and name CB)	15.00	1.41	1.42
	assign	(segid 3A4 and resid 136 and name CA)	(segid 3A4 and resid 248 and name CA)	12.04	1.15	1.15
	assign	(segid 3A4 and resid 136 and name CA)	(segid 3A4 and resid 248 and name CB)	11.87	1.11	1.11
	assign	(segid 3A4 and resid 136 and name CA)	(segid 3A4 and resid 249 and name CA)	14.02	0.87	0.87
25	assign	(segid 3A4 and resid 136 and name CA)	(segid 3A4 and resid 250 and name CA)	14.85	0.78	0.78
	assign	(segid 3A4 and resid 136 and name CA)	(segid 3A4 and resid 250 and name CB)	15.68	0.90	0.90
	assign	(segid 3A4 and resid 136 and name CA)	(segid 3A4 and resid 251 and name CA)	11.53	0.79	0.78
	assign	(segid 3A4 and resid 136 and name CA)	(segid 3A4 and resid 251 and name CB)	10.59	1.00	1.00
	assign	(segid 3A4 and resid 136 and name CA)	(segid 3A4 and resid 252 and name CA)	10.76	0.44	0.44
30	assign	(segid 3A4 and resid 136 and name CA)	(segid 3A4 and resid 252 and name CB)	10.94	0.58	0.59
	assign	(segid 3A4 and resid 136 and name CA)	(segid 3A4 and resid 253 and name CA)	14.19	0.35	0.36
	assign	(segid 3A4 and resid 136 and name CA)	(segid 3A4 and resid 253 and name CB)	14.77	0.39	0.38
	assign	(segid 3A4 and resid 136 and name CA)	(segid 3A4 and resid 254 and name CA)	12.10	1.14	1.13
	assign	(segid 3A4 and resid 136 and name CA)	(segid 3A4 and resid 255 and name CA)	12.43	0.35	0.35
35	assign	(segid 3A4 and resid 136 and name CA)	(segid 3A4 and resid 256 and name CA)	16.06	0.29	0.30
	assign	(segid 3A4 and resid 136 and name CA)	(segid 3A4 and resid 257 and name CA)	17.09	0.36	0.36
	assign	(segid 3A4 and resid 136 and name CA)	(segid 3A4 and resid 258 and name CA)	17.00	0.53	0.52
	assign	(segid 3A4 and resid 136 and name CA)	(segid 3A4 and resid 258 and name CB)	15.16	0.32	0.31
	assign	(segid 3A4 and resid 136 and name CA)	(segid 3A4 and resid 259 and name CA)	13.73	0.37	0.36
40	assign	(segid 3A4 and resid 136 and name CA)	(segid 3A4 and resid 259 and name CB)	16.16	0.25	0.26
	assign	(segid 3A4 and resid 136 and name CA)	(segid 3A4 and resid 260 and name CA)	16.03	0.35	0.35
	assign	(segid 3A4 and resid 136 and name CA)	(segid 3A4 and resid 260 and name CB)	19.12	0.44	0.43
	assign	(segid 3A4 and resid 136 and name CA)	(segid 3A4 and resid 262 and name CA)	19.06	0.23	0.24
	assign	(segid 3A4 and resid 136 and name CA)	(segid 3A4 and resid 263 and name CA)	17.80	0.23	0.23
45	assign	(segid 3A4 and resid 136 and name CA)	(segid 3A4 and resid 263 and name CB)	18.44	1.15	1.15
	assign	(segid 3A4 and resid 136 and name CA)	(segid 3A4 and resid 391 and name CA)	16.29	1.31	1.31
	assign	(segid 3A4 and resid 136 and name CA)	(segid 3A4 and resid 392 and name CA)	15.85	1.28	1.29
	assign	(segid 3A4 and resid 136 and name CA)	(segid 3A4 and resid 392 and name CB)	13.68	1.22	

	assign (segid 3A4 and resid 136 and name CB)	(segid 3A4 and resid 148 and name CA)	14.25	2.38	2.38
	assign (segid 3A4 and resid 136 and name CB)	(segid 3A4 and resid 149 and name CA)	13.53	1.73	1.74
	assign (segid 3A4 and resid 136 and name CB)	(segid 3A4 and resid 149 and name CB)	13.15	1.64	1.64
	assign (segid 3A4 and resid 136 and name CB)	(segid 3A4 and resid 152 and name CA)	16.27	1.17	1.17
	assign (segid 3A4 and resid 136 and name CB)	(segid 3A4 and resid 152 and name CB)	15.93	0.93	0.93
5	assign (segid 3A4 and resid 136 and name CB)	(segid 3A4 and resid 153 and name CA)	15.34	2.04	2.04
	assign (segid 3A4 and resid 136 and name CB)	(segid 3A4 and resid 153 and name CB)	14.51	2.47	2.48
	assign (segid 3A4 and resid 136 and name CB)	(segid 3A4 and resid 194 and name CA)	18.02	1.14	1.13
	assign (segid 3A4 and resid 136 and name CB)	(segid 3A4 and resid 194 and name CB)	17.75	1.14	1.14
	assign (segid 3A4 and resid 136 and name CB)	(segid 3A4 and resid 197 and name CA)	17.05	0.87	0.86
10	assign (segid 3A4 and resid 136 and name CB)	(segid 3A4 and resid 197 and name CB)	16.38	0.90	0.91
	assign (segid 3A4 and resid 136 and name CB)	(segid 3A4 and resid 198 and name CA)	15.36	1.02	1.02
	assign (segid 3A4 and resid 136 and name CB)	(segid 3A4 and resid 198 and name CB)	15.33	1.08	1.09
	assign (segid 3A4 and resid 136 and name CB)	(segid 3A4 and resid 201 and name CA)	14.67	0.74	0.74
	assign (segid 3A4 and resid 136 and name CB)	(segid 3A4 and resid 201 and name CB)	13.44	0.74	0.73
15	assign (segid 3A4 and resid 136 and name CB)	(segid 3A4 and resid 202 and name CA)	15.96	0.85	0.86
	assign (segid 3A4 and resid 136 and name CB)	(segid 3A4 and resid 202 and name CB)	16.63	0.95	0.95
	assign (segid 3A4 and resid 136 and name CB)	(segid 3A4 and resid 204 and name CA)	17.44	0.75	0.76
	assign (segid 3A4 and resid 136 and name CB)	(segid 3A4 and resid 204 and name CB)	16.68	0.79	0.80
	assign (segid 3A4 and resid 136 and name CB)	(segid 3A4 and resid 205 and name CA)	15.40	0.73	0.72
20	assign (segid 3A4 and resid 136 and name CB)	(segid 3A4 and resid 205 and name CB)	14.30	0.68	0.68
	assign (segid 3A4 and resid 136 and name CB)	(segid 3A4 and resid 219 and name CA)	7.65	1.01	1.01
	assign (segid 3A4 and resid 136 and name CB)	(segid 3A4 and resid 219 and name CB)	7.25	0.86	0.85
	assign (segid 3A4 and resid 136 and name CB)	(segid 3A4 and resid 220 and name CA)	8.93	1.30	1.30
	assign (segid 3A4 and resid 136 and name CB)	(segid 3A4 and resid 220 and name CB)	8.52	1.34	1.33
25	assign (segid 3A4 and resid 136 and name CB)	(segid 3A4 and resid 221 and name CA)	11.03	0.90	0.89
	assign (segid 3A4 and resid 136 and name CB)	(segid 3A4 and resid 221 and name CB)	10.84	0.69	0.69
	assign (segid 3A4 and resid 136 and name CB)	(segid 3A4 and resid 222 and name CA)	12.65	0.90	0.91
	assign (segid 3A4 and resid 136 and name CB)	(segid 3A4 and resid 222 and name CB)	12.28	0.81	0.80
	assign (segid 3A4 and resid 136 and name CB)	(segid 3A4 and resid 223 and name CA)	13.47	1.27	1.26
30	assign (segid 3A4 and resid 136 and name CB)	(segid 3A4 and resid 223 and name CB)	12.70	1.33	1.34
	assign (segid 3A4 and resid 136 and name CB)	(segid 3A4 and resid 224 and name CA)	14.98	1.25	1.25
	assign (segid 3A4 and resid 136 and name CB)	(segid 3A4 and resid 224 and name CB)	14.49	1.21	1.21
	assign (segid 3A4 and resid 136 and name CB)	(segid 3A4 and resid 225 and name CA)	16.80	0.99	0.99
	assign (segid 3A4 and resid 136 and name CB)	(segid 3A4 and resid 225 and name CB)	16.34	0.87	0.88
35	assign (segid 3A4 and resid 136 and name CB)	(segid 3A4 and resid 226 and name CA)	18.40	1.13	1.12
	assign (segid 3A4 and resid 136 and name CB)	(segid 3A4 and resid 244 and name CA)	17.46	1.69	1.68
	assign (segid 3A4 and resid 136 and name CB)	(segid 3A4 and resid 244 and name CB)	17.43	1.64	1.65
	assign (segid 3A4 and resid 136 and name CB)	(segid 3A4 and resid 245 and name CA)	17.25	1.54	1.55
	assign (segid 3A4 and resid 136 and name CB)	(segid 3A4 and resid 247 and name CA)	15.85	1.77	1.76
40	assign (segid 3A4 and resid 136 and name CB)	(segid 3A4 and resid 247 and name CB)	15.75	1.87	1.87
	assign (segid 3A4 and resid 136 and name CB)	(segid 3A4 and resid 248 and name CA)	12.95	1.52	1.53
	assign (segid 3A4 and resid 136 and name CB)	(segid 3A4 and resid 248 and name CB)	12.91	1.44	1.44
	assign (segid 3A4 and resid 136 and name CB)	(segid 3A4 and resid 249 and name CA)	14.85	1.19	1.19
	assign (segid 3A4 and resid 136 and name CB)	(segid 3A4 and resid 250 and name CA)	15.41	1.25	1.25
45	assign (segid 3A4 and resid 136 and name CB)	(segid 3A4 and resid 250 and name CB)	16.21	1.39	1.39
	assign (segid 3A4 and resid 136 and name CB)	(segid 3A4 and resid 251 and name CA)	11.95	1.31	1.32
	assign (segid 3A4 and resid 136 and name CB)	(segid 3A4 and resid 251 and name CB)	11.07	1.53	1.53
	assign (segid 3A4 and resid 136 and name CB)	(segid 3A4 and resid 252 and name CA)	11.31	0.69	0.70
	assign (segid 3A4 and resid 136 and name CB)	(segid 3A4 and resid 252 and name CB)	11.64	0.72	0.72
50	assign (segid 3A4 and resid 136 and name CB)	(segid 3A4 and resid 253 and name CA)	14.58	0.52	0.53
	assign (segid 3A4 and resid 136 and name CB)	(segid 3A4 and resid 254 and name CA)	14.90	0.84	0.83
	assign (segid 3A4 and resid 136 and name CB)	(segid 3A4 and resid 255 and name CA)	12.05	1.38	1.37
	assign (segid 3A4 and resid 136 and name CB)	(segid 3A4 and resid 256 and name CA)	12.41	0.52	0.52
	assign (segid 3A4 and resid 136 and name CB)	(segid 3A4 and resid 257 and name CA)	15.97	0.40	0.41
55	assign (segid 3A4 and resid 136 and name CB)	(segid 3A4 and resid 258 and name CA)	16.78	0.69	0.70
	assign (segid 3A4 and resid 136 and name CB)	(segid 3A4 and resid 258 and name CB)	16.70	0.91	0.90
	assign (segid 3A4 and resid 136 and name CB)	(segid 3A4 and resid 259 and name CA)	14.63	0.62	0.62
	assign (segid 3A4 and resid 136 and name CB)	(segid 3A4 and resid 259 and name CB)	13.18	0.64	0.65
	assign (segid 3A4 and resid 136 and name CB)	(segid 3A4 and resid 260 and name CA)	15.72	0.40	0.39
60	assign (segid 3A4 and resid 136 and name CB)	(segid 3A4 and resid 260 and name CB)	15.69	0.46	0.46
	assign (segid 3A4 and resid 136 and name CB)	(segid 3A4 and resid 261 and name CA)	19.25	0.45	0.44
	assign (segid 3A4 and resid 136 and name CB)	(segid 3A4 and resid 262 and name CA)	19.24	0.57	0.57
	assign (segid 3A4 and resid 136 and name CB)	(segid 3A4 and resid 262 and name CB)	18.45	0.68	0.69
	assign (segid 3A4 and resid 136 and name CB)	(segid 3A4 and resid 263 and name CA)	18.31	0.36	0.37
65	assign (segid 3A4 and resid 136 and name CB)	(segid 3A4 and resid 263 and name CB)	17.05	0.34	0.35
	assign (segid 3A4 and resid 136 and name CB)	(segid 3A4 and resid 392 and name CA)	16.04	1.87	1.87
	assign (segid 3A4 and resid 136 and name CB)	(segid 3A4 and resid 392 and name CB)	15.73	1.85	1.85
	assign (segid 3A4 and resid 136 and name CB)	(segid 3A4 and resid 393 and name CA)	13.26	1.75	1.75
	assign (segid 3A4 and resid 136 and name CB)	(segid 3A4 and resid 394 and name CA)	15.82	1.62	1.61
70	assign (segid 3A4 and resid 136 and name CB)	(segid 3A4 and resid 394 and name CB)	17.21	1.69	1.69
	assign (segid 3A4 and resid 136 and name CB)	(segid 3A4 and resid 395 and name CA)	14.54	1.66	1.66
	assign (segid 3A4 and resid 136 and name CB)	(segid 3A4 and resid 396 and name CA)	11.09	1.52	1.51
	assign (segid 3A4 and resid 136 and name CB)	(segid 3A4 and resid 396 and name CB)	10.03	1.60	1.61
	assign (segid 3A4 and resid 136 and name CB)	(segid 3A4 and resid 397 and name CA)	13.05	1.38	1.38
75	assign (segid 3A4 and resid 136 and name CB)	(segid 3A4 and resid 397 and name CB)	14.04	1.43	1.44
	assign (segid 3A4 and resid 136 and name CB)	(segid 3A4 and resid 398 and name CA)	15.56	1.30	1.30
	assign (segid 3A4 and resid 136 and name CB)	(segid 3A4 and resid 398 and name CB)	16.54	1.38	1.38
	assign (segid 3A4 and resid 136 and name CB)	(segid 3A4 and resid 399 and name CA)	13.47	1.10	1.09
	assign (segid 3A4 and resid 136 and name CB)	(segid 3A4 and resid 399 and name CB)	12.51	1.12	1.12
80	assign (segid 3A4 and resid 136 and name CB)	(segid 3A4 and resid 400 and name CA)	11.90	1.01	1.02
	assign (segid 3A4 and resid 136 and name CB)	(segid 3A4 and resid 400 and name CB)	11.10	1.08	1.08
	assign (segid 3A4 and resid 136 and name CB)	(segid 3A4 and resid 401 and name CA)	15.44	1.06	1.06

	assign (segid 3A4 and resid 136 and name CB)	(segid 3A4 and resid 402 and name CA)	17.11	0.97	0.97
	assign (segid 3A4 and resid 136 and name CB)	(segid 3A4 and resid 402 and name CB)	17.30	0.98	0.98
	assign (segid 3A4 and resid 136 and name CB)	(segid 3A4 and resid 403 and name CA)	15.11	0.78	0.77
	assign (segid 3A4 and resid 136 and name CB)	(segid 3A4 and resid 403 and name CB)	13.69	0.75	0.75
	assign (segid 3A4 and resid 136 and name CB)	(segid 3A4 and resid 404 and name CA)	15.55	0.82	0.83
5	assign (segid 3A4 and resid 136 and name CB)	(segid 3A4 and resid 404 and name CB)	15.15	0.91	0.91
	assign (segid 3A4 and resid 136 and name CB)	(segid 3A4 and resid 407 and name CA)	18.93	0.71	0.71
	assign (segid 3A4 and resid 136 and name CB)	(segid 3A4 and resid 407 and name CB)	17.57	0.70	0.71
	assign (segid 3A4 and resid 136 and name N)	(segid 3A4 and resid 136 and name C)	2.47	0.02	0.02
	assign (segid 3A4 and resid 136 and name N)	(segid 3A4 and resid 136 and name CA)	1.46	0.00	0.01
10	assign (segid 3A4 and resid 136 and name N)	(segid 3A4 and resid 136 and name CB)	2.47	0.03	0.04
	assign (segid 3A4 and resid 136 and name N)	(segid 3A4 and resid 136 and name O)	3.54	0.04	0.05
	assign (segid 3A4 and resid 136 and name N)	(segid 3A4 and resid 137 and name C)	4.77	0.09	0.10
	assign (segid 3A4 and resid 136 and name N)	(segid 3A4 and resid 137 and name CA)	4.21	0.07	0.06
	assign (segid 3A4 and resid 136 and name N)	(segid 3A4 and resid 137 and name N)	2.79	0.07	0.07
15	assign (segid 3A4 and resid 136 and name N)	(segid 3A4 and resid 137 and name O)	5.84	0.12	0.13
	assign (segid 3A4 and resid 136 and name N)	(segid 3A4 and resid 138 and name C)	5.67	0.17	0.17
	assign (segid 3A4 and resid 136 and name N)	(segid 3A4 and resid 138 and name CA)	5.50	0.25	0.26
	assign (segid 3A4 and resid 136 and name N)	(segid 3A4 and resid 138 and name CB)	5.90	0.54	0.55
	assign (segid 3A4 and resid 136 and name N)	(segid 3A4 and resid 138 and name N)	4.45	0.20	0.19
20	assign (segid 3A4 and resid 136 and name N)	(segid 3A4 and resid 138 and name O)	6.80	0.16	0.17
	assign (segid 3A4 and resid 136 and name N)	(segid 3A4 and resid 139 and name C)	5.79	0.17	0.18
	assign (segid 3A4 and resid 136 and name N)	(segid 3A4 and resid 139 and name CA)	5.40	0.08	0.08
	assign (segid 3A4 and resid 136 and name N)	(segid 3A4 and resid 139 and name N)	4.79	0.10	0.09
	assign (segid 3A4 and resid 136 and name N)	(segid 3A4 and resid 139 and name O)	6.80	0.22	0.23
25	assign (segid 3A4 and resid 136 and name N)	(segid 3A4 and resid 140 and name C)	6.05	0.49	0.50
	assign (segid 3A4 and resid 136 and name N)	(segid 3A4 and resid 140 and name CA)	6.18	0.61	0.62
	assign (segid 3A4 and resid 136 and name N)	(segid 3A4 and resid 140 and name N)	5.37	0.46	0.46
	assign (segid 3A4 and resid 136 and name N)	(segid 3A4 and resid 140 and name O)	5.13	0.47	0.48
	assign (segid 3A4 and resid 136 and name N)	(segid 3A4 and resid 136 and name CB)	3.19	0.12	0.11
30	assign (segid 3A4 and resid 136 and name O)	(segid 3A4 and resid 137 and name C)	3.14	0.28	0.28
	assign (segid 3A4 and resid 136 and name O)	(segid 3A4 and resid 137 and name CA)	2.74	0.03	0.04
	assign (segid 3A4 and resid 136 and name O)	(segid 3A4 and resid 137 and name N)	2.23	0.01	0.02
	assign (segid 3A4 and resid 136 and name O)	(segid 3A4 and resid 137 and name O)	3.60	0.35	0.35
	assign (segid 3A4 and resid 136 and name O)	(segid 3A4 and resid 138 and name C)	4.80	0.63	0.64
35	assign (segid 3A4 and resid 136 and name O)	(segid 3A4 and resid 138 and name CA)	4.75	0.44	0.43
	assign (segid 3A4 and resid 136 and name O)	(segid 3A4 and resid 138 and name CB)	5.86	0.48	0.47
	assign (segid 3A4 and resid 136 and name O)	(segid 3A4 and resid 138 and name N)	3.71	0.36	0.35
	assign (segid 3A4 and resid 136 and name O)	(segid 3A4 and resid 138 and name O)	5.84	0.64	0.64
	assign (segid 3A4 and resid 136 and name O)	(segid 3A4 and resid 139 and name C)	5.84	0.95	0.96
40	assign (segid 3A4 and resid 136 and name O)	(segid 3A4 and resid 139 and name CA)	4.73	0.84	0.85
	assign (segid 3A4 and resid 136 and name O)	(segid 3A4 and resid 139 and name N)	4.08	0.78	0.77
	assign (segid 3A4 and resid 136 and name O)	(segid 3A4 and resid 140 and name N)	6.05	1.01	1.01
	assign (segid 3A4 and resid 136 and name O)	(segid 3A4 and resid 219 and name C)	5.38	1.01	1.00
45	assign (segid 3A4 and resid 136 and name O)	(segid 3A4 and resid 219 and name CA)	4.69	0.75	0.75
	assign (segid 3A4 and resid 136 and name O)	(segid 3A4 and resid 219 and name CB)	4.25	0.59	0.58
	assign (segid 3A4 and resid 136 and name O)	(segid 3A4 and resid 219 and name CG)	5.46	0.63	0.63
	assign (segid 3A4 and resid 136 and name O)	(segid 3A4 and resid 219 and name N)	5.82	0.63	0.62
	assign (segid 3A4 and resid 136 and name O)	(segid 3A4 and resid 219 and name O)	6.58	1.01	1.00
50	assign (segid 3A4 and resid 136 and name O)	(segid 3A4 and resid 220 and name CA)	6.07	1.20	1.20
	assign (segid 3A4 and resid 136 and name O)	(segid 3A4 and resid 220 and name CB)	5.94	1.24	1.24
	assign (segid 3A4 and resid 136 and name O)	(segid 3A4 and resid 220 and name N)	4.94	1.13	1.14
	assign (segid 3A4 and resid 136 and name O)	(segid 3A4 and resid 137 and name O)	1.23	0.00	0.01
	assign (segid 3A4 and resid 137 and name C)	(segid 3A4 and resid 138 and name C)	3.31	0.15	0.16
	assign (segid 3A4 and resid 137 and name C)	(segid 3A4 and resid 138 and name CA)	2.43	0.01	0.02
55	assign (segid 3A4 and resid 137 and name C)	(segid 3A4 and resid 138 and name CB)	3.56	0.14	0.15
	assign (segid 3A4 and resid 137 and name C)	(segid 3A4 and resid 138 and name N)	1.32	0.01	0.02
	assign (segid 3A4 and resid 137 and name C)	(segid 3A4 and resid 138 and name O)	4.31	0.23	0.23
	assign (segid 3A4 and resid 137 and name C)	(segid 3A4 and resid 139 and name C)	5.91	0.15	0.15
	assign (segid 3A4 and resid 137 and name C)	(segid 3A4 and resid 139 and name CA)	4.81	0.20	0.20
60	assign (segid 3A4 and resid 137 and name C)	(segid 3A4 and resid 139 and name N)	3.51	0.17	0.16
	assign (segid 3A4 and resid 137 and name C)	(segid 3A4 and resid 139 and name O)	7.01	0.17	0.18
	assign (segid 3A4 and resid 137 and name C)	(segid 3A4 and resid 140 and name CA)	7.20	0.05	0.05
	assign (segid 3A4 and resid 137 and name C)	(segid 3A4 and resid 140 and name CB)	7.35	0.16	0.16
	assign (segid 3A4 and resid 137 and name C)	(segid 3A4 and resid 140 and name N)	5.91	0.07	0.06
65	assign (segid 3A4 and resid 137 and name C)	(segid 3A4 and resid 140 and name O)	7.34	0.29	0.30
	assign (segid 3A4 and resid 137 and name C)	(segid 3A4 and resid 219 and name C)	4.94	0.09	0.09
	assign (segid 3A4 and resid 137 and name C)	(segid 3A4 and resid 219 and name CA)	4.83	0.15	0.16
	assign (segid 3A4 and resid 137 and name C)	(segid 3A4 and resid 219 and name CB)	4.32	0.19	0.18
	assign (segid 3A4 and resid 137 and name C)	(segid 3A4 and resid 219 and name CG)	5.14	0.63	0.62
70	assign (segid 3A4 and resid 137 and name C)	(segid 3A4 and resid 219 and name N)	6.17	0.10	0.09
	assign (segid 3A4 and resid 137 and name C)	(segid 3A4 and resid 219 and name O)	6.04	0.11	0.10
	assign (segid 3A4 and resid 137 and name C)	(segid 3A4 and resid 220 and name C)	5.62	0.29	0.29
	assign (segid 3A4 and resid 137 and name C)	(segid 3A4 and resid 220 and name CA)	4.89	0.13	0.13
	assign (segid 3A4 and resid 137 and name C)	(segid 3A4 and resid 220 and name CB)	4.44	0.11	0.11
75	assign (segid 3A4 and resid 137 and name C)	(segid 3A4 and resid 220 and name N)	4.18	0.20	0.21
	assign (segid 3A4 and resid 137 and name C)	(segid 3A4 and resid 220 and name O)	6.79	0.27	0.28
	assign (segid 3A4 and resid 137 and name C)	(segid 3A4 and resid 221 and name CA)	6.35	0.67	0.68
	assign (segid 3A4 and resid 137 and name C)	(segid 3A4 and resid 221 and name CB)	6.19	0.86	0.86
	assign (segid 3A4 and resid 137 and name C)	(segid 3A4 and resid 221 and name N)	5.25	0.52	0.51
80	assign (segid 3A4 and resid 137 and name C)	(segid 3A4 and resid 222 and name N)	7.39	0.54	0.54
	assign (segid 3A4 and resid 137 and name C)	(segid 3A4 and resid 137 and name C)	1.53	0.01	0.01
	assign (segid 3A4 and resid 137 and name CA)	(segid 3A4 and resid 137 and name O)	2.40	0.00	0.01

	assign (segid 3A4 and resid 137 and name CA) (segid 3A4 and resid 138 and name C)	4.64	0.11	0.12
	assign (segid 3A4 and resid 137 and name CA) (segid 3A4 and resid 138 and name CA)	3.81	0.02	0.02
	assign (segid 3A4 and resid 137 and name CA) (segid 3A4 and resid 138 and name CB)	4.74	0.11	0.11
	assign (segid 3A4 and resid 137 and name CA) (segid 3A4 and resid 138 and name N)	2.44	0.03	0.02
	assign (segid 3A4 and resid 137 and name CA) (segid 3A4 and resid 138 and name O)	5.70	0.19	0.19
5	assign (segid 3A4 and resid 137 and name CA) (segid 3A4 and resid 139 and name C)	6.79	0.14	0.14
	assign (segid 3A4 and resid 137 and name CA) (segid 3A4 and resid 139 and name CA)	5.74	0.16	0.16
	assign (segid 3A4 and resid 137 and name CA) (segid 3A4 and resid 139 and name N)	4.55	0.12	0.12
	assign (segid 3A4 and resid 137 and name CA) (segid 3A4 and resid 140 and name CA)	7.93	0.15	0.15
	assign (segid 3A4 and resid 137 and name CA) (segid 3A4 and resid 140 and name CB)	8.09	0.27	0.26
10	assign (segid 3A4 and resid 137 and name CA) (segid 3A4 and resid 140 and name N)	6.70	0.13	0.13
	assign (segid 3A4 and resid 137 and name CA) (segid 3A4 and resid 141 and name CA)	10.32	0.31	0.31
	assign (segid 3A4 and resid 137 and name CA) (segid 3A4 and resid 141 and name CB)	11.45	0.47	0.47
	assign (segid 3A4 and resid 137 and name CA) (segid 3A4 and resid 147 and name CA)	14.05	2.61	2.62
	assign (segid 3A4 and resid 137 and name CA) (segid 3A4 and resid 148 and name CA)	15.15	0.57	0.56
15	assign (segid 3A4 and resid 137 and name CA) (segid 3A4 and resid 149 and name CA)	14.08	0.28	0.28
	assign (segid 3A4 and resid 137 and name CA) (segid 3A4 and resid 149 and name CB)	13.57	0.39	0.40
	assign (segid 3A4 and resid 137 and name CA) (segid 3A4 and resid 150 and name CA)	14.52	1.93	1.92
	assign (segid 3A4 and resid 137 and name CA) (segid 3A4 and resid 151 and name CA)	16.79	0.89	0.88
	assign (segid 3A4 and resid 137 and name CA) (segid 3A4 and resid 152 and name CA)	16.32	1.08	1.08
20	assign (segid 3A4 and resid 137 and name CA) (segid 3A4 and resid 152 and name CB)	15.94	1.58	1.59
	assign (segid 3A4 and resid 137 and name CA) (segid 3A4 and resid 153 and name CA)	15.22	1.17	1.16
	assign (segid 3A4 and resid 137 and name CA) (segid 3A4 and resid 153 and name CB)	14.44	1.66	1.66
	assign (segid 3A4 and resid 137 and name CA) (segid 3A4 and resid 156 and name CA)	18.05	1.33	1.32
	assign (segid 3A4 and resid 137 and name CA) (segid 3A4 and resid 156 and name CB)	17.15	1.49	1.49
25	assign (segid 3A4 and resid 137 and name CA) (segid 3A4 and resid 194 and name CA)	16.15	1.44	1.43
	assign (segid 3A4 and resid 137 and name CA) (segid 3A4 and resid 194 and name CB)	15.87	1.31	1.30
	assign (segid 3A4 and resid 137 and name CA) (segid 3A4 and resid 195 and name CA)	16.86	1.56	1.56
	assign (segid 3A4 and resid 137 and name CA) (segid 3A4 and resid 197 and name CA)	15.20	1.52	1.52
	assign (segid 3A4 and resid 137 and name CA) (segid 3A4 and resid 197 and name CB)	14.74	1.45	1.45
30	assign (segid 3A4 and resid 137 and name CA) (segid 3A4 and resid 198 and name CA)	12.81	1.70	1.71
	assign (segid 3A4 and resid 137 and name CA) (segid 3A4 and resid 198 and name CB)	12.62	1.70	1.69
	assign (segid 3A4 and resid 137 and name CA) (segid 3A4 and resid 199 and name CA)	15.57	1.82	1.81
	assign (segid 3A4 and resid 137 and name CA) (segid 3A4 and resid 199 and name CB)	16.99	1.83	1.83
	assign (segid 3A4 and resid 137 and name CA) (segid 3A4 and resid 200 and name CA)	15.86	1.52	1.51
35	assign (segid 3A4 and resid 137 and name CA) (segid 3A4 and resid 201 and name CA)	12.34	1.40	1.40
	assign (segid 3A4 and resid 137 and name CA) (segid 3A4 and resid 201 and name CB)	11.09	1.45	1.46
	assign (segid 3A4 and resid 137 and name CA) (segid 3A4 and resid 202 and name CA)	12.94	1.51	1.51
	assign (segid 3A4 and resid 137 and name CA) (segid 3A4 and resid 202 and name CB)	13.44	1.60	1.60
	assign (segid 3A4 and resid 137 and name CA) (segid 3A4 and resid 203 and name CA)	16.27	1.39	1.38
40	assign (segid 3A4 and resid 137 and name CA) (segid 3A4 and resid 203 and name CB)	17.33	1.41	1.40
	assign (segid 3A4 and resid 137 and name CA) (segid 3A4 and resid 204 and name CA)	15.28	1.06	1.05
	assign (segid 3A4 and resid 137 and name CA) (segid 3A4 and resid 204 and name CB)	14.75	0.91	0.91
	assign (segid 3A4 and resid 137 and name CA) (segid 3A4 and resid 205 and name CA)	12.87	1.07	1.06
	assign (segid 3A4 and resid 137 and name CA) (segid 3A4 and resid 205 and name CB)	11.58	1.08	1.08
45	assign (segid 3A4 and resid 137 and name CA) (segid 3A4 and resid 206 and name CA)	15.85	1.08	1.09
	assign (segid 3A4 and resid 137 and name CA) (segid 3A4 and resid 206 and name CB)	16.66	1.15	1.14
	assign (segid 3A4 and resid 137 and name CA) (segid 3A4 and resid 207 and name CA)	18.04	0.96	0.96
	assign (segid 3A4 and resid 137 and name CA) (segid 3A4 and resid 207 and name CB)	18.61	1.00	1.00
50	assign (segid 3A4 and resid 137 and name CA) (segid 3A4 and resid 219 and name C)	5.71	0.35	0.34
	assign (segid 3A4 and resid 137 and name CA) (segid 3A4 and resid 219 and name CA)	5.51	0.18	0.18
	assign (segid 3A4 and resid 137 and name CA) (segid 3A4 and resid 219 and name CB)	5.19	0.46	0.45
	assign (segid 3A4 and resid 137 and name CA) (segid 3A4 and resid 219 and name CG)	6.23	0.78	0.78
	assign (segid 3A4 and resid 137 and name CA) (segid 3A4 and resid 219 and name N)	6.81	0.15	0.14
	assign (segid 3A4 and resid 137 and name CA) (segid 3A4 and resid 219 and name O)	6.85	0.43	0.43
55	assign (segid 3A4 and resid 137 and name CA) (segid 3A4 and resid 220 and name C)	6.56	0.68	0.68
	assign (segid 3A4 and resid 137 and name CA) (segid 3A4 and resid 220 and name CA)	5.60	0.48	0.47
	assign (segid 3A4 and resid 137 and name CA) (segid 3A4 and resid 220 and name CB)	4.97	0.53	0.53
	assign (segid 3A4 and resid 137 and name CA) (segid 3A4 and resid 220 and name N)	4.91	0.36	0.35
	assign (segid 3A4 and resid 137 and name CA) (segid 3A4 and resid 221 and name CA)	7.59	0.95	0.95
60	assign (segid 3A4 and resid 137 and name CA) (segid 3A4 and resid 221 and name CB)	7.55	1.04	1.04
	assign (segid 3A4 and resid 137 and name CA) (segid 3A4 and resid 221 and name N)	6.37	0.86	0.86
	assign (segid 3A4 and resid 137 and name CA) (segid 3A4 and resid 222 and name CA)	9.79	0.70	0.69
	assign (segid 3A4 and resid 137 and name CA) (segid 3A4 and resid 222 and name CB)	9.75	0.57	0.58
	assign (segid 3A4 and resid 137 and name CA) (segid 3A4 and resid 223 and name CA)	10.42	0.47	0.47
65	assign (segid 3A4 and resid 137 and name CA) (segid 3A4 and resid 223 and name CB)	9.72	0.32	0.31
	assign (segid 3A4 and resid 137 and name CA) (segid 3A4 and resid 224 and name CA)	11.44	0.76	0.76
	assign (segid 3A4 and resid 137 and name CA) (segid 3A4 and resid 224 and name CB)	10.81	0.85	0.85
	assign (segid 3A4 and resid 137 and name CA) (segid 3A4 and resid 225 and name CA)	13.44	0.87	0.87
	assign (segid 3A4 and resid 137 and name CA) (segid 3A4 and resid 225 and name CB)	13.13	0.90	0.89
70	assign (segid 3A4 and resid 137 and name CA) (segid 3A4 and resid 226 and name CA)	15.30	0.68	0.68
	assign (segid 3A4 and resid 137 and name CA) (segid 3A4 and resid 241 and name CA)	17.80	1.86	1.85
	assign (segid 3A4 and resid 137 and name CA) (segid 3A4 and resid 243 and name CA)	17.09	1.60	1.61
	assign (segid 3A4 and resid 137 and name CA) (segid 3A4 and resid 243 and name CB)	17.65	1.55	1.54
	assign (segid 3A4 and resid 137 and name CA) (segid 3A4 and resid 244 and name CA)	13.79	1.70	1.70
75	assign (segid 3A4 and resid 137 and name CA) (segid 3A4 and resid 244 and name CB)	13.77	1.75	1.75
	assign (segid 3A4 and resid 137 and name CA) (segid 3A4 and resid 245 and name CA)	13.87	1.85	1.85
	assign (segid 3A4 and resid 137 and name CA) (segid 3A4 and resid 245 and name CB)	15.10	1.87	1.87
	assign (segid 3A4 and resid 137 and name CA) (segid 3A4 and resid 246 and name CA)	15.04	1.58	1.58
	assign (segid 3A4 and resid 137 and name CA) (segid 3A4 and resid 246 and name CB)	16.36	1.59	1.59
80	assign (segid 3A4 and resid 137 and name CA) (segid 3A4 and resid 247 and name CA)	12.42	1.47	1.48
	assign (segid 3A4 and resid 137 and name CA) (segid 3A4 and resid 247 and name CB)	12.21	1.49	1.49
	assign (segid 3A4 and resid 137 and name CA) (segid 3A4 and resid 248 and name CA)	9.64	1.54	1.55

	assign (segid 3A4 and resid 137 and name CA)	(segid 3A4 and resid 248 and name CB)	9.57	1.66	1.67
	assign (segid 3A4 and resid 137 and name CA)	(segid 3A4 and resid 249 and name CA)	12.12	1.28	1.28
	assign (segid 3A4 and resid 137 and name CA)	(segid 3A4 and resid 250 and name CA)	12.74	0.97	0.96
	assign (segid 3A4 and resid 137 and name CA)	(segid 3A4 and resid 250 and name CB)	13.38	1.01	1.02
5	assign (segid 3A4 and resid 137 and name CA)	(segid 3A4 and resid 251 and name CA)	9.42	0.71	0.72
	assign (segid 3A4 and resid 137 and name CA)	(segid 3A4 and resid 251 and name CB)	8.28	0.85	0.85
	assign (segid 3A4 and resid 137 and name CA)	(segid 3A4 and resid 252 and name CA)	9.48	0.54	0.55
	assign (segid 3A4 and resid 137 and name CA)	(segid 3A4 and resid 252 and name CB)	9.77	0.70	0.69
	assign (segid 3A4 and resid 137 and name CA)	(segid 3A4 and resid 253 and name CA)	13.03	0.48	0.47
10	assign (segid 3A4 and resid 137 and name CA)	(segid 3A4 and resid 254 and name CA)	13.32	0.60	0.61
	assign (segid 3A4 and resid 137 and name CA)	(segid 3A4 and resid 255 and name CA)	11.09	1.24	1.24
	assign (segid 3A4 and resid 137 and name CA)	(segid 3A4 and resid 256 and name CA)	12.19	0.50	0.51
	assign (segid 3A4 and resid 137 and name CA)	(segid 3A4 and resid 257 and name CA)	15.85	0.52	0.52
	assign (segid 3A4 and resid 137 and name CA)	(segid 3A4 and resid 258 and name CA)	16.62	0.62	0.62
15	assign (segid 3A4 and resid 137 and name CA)	(segid 3A4 and resid 258 and name CB)	16.28	0.68	0.68
	assign (segid 3A4 and resid 137 and name CA)	(segid 3A4 and resid 259 and name CA)	15.14	0.60	0.60
	assign (segid 3A4 and resid 137 and name CA)	(segid 3A4 and resid 259 and name CB)	13.74	0.62	0.61
	assign (segid 3A4 and resid 137 and name CA)	(segid 3A4 and resid 260 and name CA)	16.70	0.51	0.51
	assign (segid 3A4 and resid 137 and name CA)	(segid 3A4 and resid 260 and name CB)	16.60	0.51	0.50
20	assign (segid 3A4 and resid 137 and name CA)	(segid 3A4 and resid 391 and name CA)	16.76	0.54	0.54
	assign (segid 3A4 and resid 137 and name CA)	(segid 3A4 and resid 391 and name CB)	16.70	0.54	0.53
	assign (segid 3A4 and resid 137 and name CA)	(segid 3A4 and resid 392 and name CA)	14.08	0.45	0.45
	assign (segid 3A4 and resid 137 and name CA)	(segid 3A4 and resid 392 and name CB)	13.47	0.42	0.42
	assign (segid 3A4 and resid 137 and name CA)	(segid 3A4 and resid 393 and name CA)	11.93	0.51	0.52
25	assign (segid 3A4 and resid 137 and name CA)	(segid 3A4 and resid 394 and name CA)	15.08	0.63	0.62
	assign (segid 3A4 and resid 137 and name CA)	(segid 3A4 and resid 394 and name CB)	16.38	0.58	0.57
	assign (segid 3A4 and resid 137 and name CA)	(segid 3A4 and resid 395 and name CA)	14.21	0.75	0.74
	assign (segid 3A4 and resid 137 and name CA)	(segid 3A4 and resid 396 and name CA)	11.08	0.89	0.90
	assign (segid 3A4 and resid 137 and name CA)	(segid 3A4 and resid 396 and name CB)	9.76	0.84	0.83
30	assign (segid 3A4 and resid 137 and name CA)	(segid 3A4 and resid 397 and name CA)	13.30	0.77	0.76
	assign (segid 3A4 and resid 137 and name CA)	(segid 3A4 and resid 397 and name CB)	14.04	0.68	0.68
	assign (segid 3A4 and resid 137 and name CA)	(segid 3A4 and resid 398 and name CA)	16.18	0.88	0.88
	assign (segid 3A4 and resid 137 and name CA)	(segid 3A4 and resid 398 and name CB)	17.00	0.83	0.84
	assign (segid 3A4 and resid 137 and name CA)	(segid 3A4 and resid 399 and name CA)	14.60	1.03	1.02
35	assign (segid 3A4 and resid 137 and name CA)	(segid 3A4 and resid 399 and name CB)	13.54	1.03	1.03
	assign (segid 3A4 and resid 137 and name CA)	(segid 3A4 and resid 400 and name CA)	13.48	1.04	1.03
	assign (segid 3A4 and resid 137 and name CA)	(segid 3A4 and resid 400 and name CB)	12.53	1.08	1.08
	assign (segid 3A4 and resid 137 and name CA)	(segid 3A4 and resid 401 and name CA)	16.94	1.03	1.03
	assign (segid 3A4 and resid 137 and name CA)	(segid 3A4 and resid 403 and name CA)	17.38	1.00	0.99
40	assign (segid 3A4 and resid 137 and name CA)	(segid 3A4 and resid 403 and name CB)	16.00	1.02	1.02
	assign (segid 3A4 and resid 137 and name CA)	(segid 3A4 and resid 404 and name CA)	17.96	0.81	0.81
	assign (segid 3A4 and resid 137 and name CA)	(segid 3A4 and resid 404 and name CB)	17.41	0.79	0.79
	assign (segid 3A4 and resid 137 and name N)	(segid 3A4 and resid 137 and name C)	2.46	0.03	0.04
	assign (segid 3A4 and resid 137 and name N)	(segid 3A4 and resid 137 and name O)	1.45	0.01	0.02
45	assign (segid 3A4 and resid 137 and name N)	(segid 3A4 and resid 138 and name C)	3.49	0.05	0.06
	assign (segid 3A4 and resid 137 and name N)	(segid 3A4 and resid 138 and name CA)	4.82	0.12	0.12
	assign (segid 3A4 and resid 137 and name N)	(segid 3A4 and resid 138 and name CB)	4.22	0.08	0.08
	assign (segid 3A4 and resid 137 and name N)	(segid 3A4 and resid 138 and name N)	5.02	0.15	0.15
	assign (segid 3A4 and resid 137 and name N)	(segid 3A4 and resid 138 and name O)	2.81	0.09	0.10
50	assign (segid 3A4 and resid 137 and name N)	(segid 3A4 and resid 139 and name C)	5.98	0.15	0.15
	assign (segid 3A4 and resid 137 and name N)	(segid 3A4 and resid 139 and name CA)	6.33	0.16	0.15
	assign (segid 3A4 and resid 137 and name N)	(segid 3A4 and resid 139 and name N)	5.43	0.12	0.11
	assign (segid 3A4 and resid 137 and name N)	(segid 3A4 and resid 139 and name O)	4.38	0.11	0.10
	assign (segid 3A4 and resid 137 and name N)	(segid 3A4 and resid 139 and name O)	7.45	0.19	0.19
55	assign (segid 3A4 and resid 137 and name N)	(segid 3A4 and resid 140 and name C)	7.53	0.23	0.22
	assign (segid 3A4 and resid 137 and name N)	(segid 3A4 and resid 140 and name CA)	7.30	0.24	0.24
	assign (segid 3A4 and resid 137 and name N)	(segid 3A4 and resid 140 and name N)	6.15	0.20	0.20
	assign (segid 3A4 and resid 137 and name N)	(segid 3A4 and resid 140 and name O)	6.75	0.26	0.26
	assign (segid 3A4 and resid 137 and name N)	(segid 3A4 and resid 219 and name C)	6.51	0.64	0.64
60	assign (segid 3A4 and resid 137 and name N)	(segid 3A4 and resid 219 and name CA)	6.08	0.54	0.54
	assign (segid 3A4 and resid 137 and name N)	(segid 3A4 and resid 219 and name CB)	5.58	0.67	0.68
	assign (segid 3A4 and resid 137 and name N)	(segid 3A4 and resid 219 and name CG)	6.69	0.86	0.86
	assign (segid 3A4 and resid 137 and name N)	(segid 3A4 and resid 219 and name N)	7.33	0.49	0.48
	assign (segid 3A4 and resid 137 and name N)	(segid 3A4 and resid 220 and name CA)	6.64	0.69	0.68
65	assign (segid 3A4 and resid 137 and name N)	(segid 3A4 and resid 220 and name CB)	6.06	0.70	0.70
	assign (segid 3A4 and resid 137 and name N)	(segid 3A4 and resid 220 and name N)	5.81	0.65	0.64
	assign (segid 3A4 and resid 137 and name N)	(segid 3A4 and resid 138 and name C)	3.48	0.27	0.28
	assign (segid 3A4 and resid 137 and name N)	(segid 3A4 and resid 138 and name CA)	2.77	0.05	0.04
	assign (segid 3A4 and resid 137 and name N)	(segid 3A4 and resid 138 and name CB)	4.02	0.26	0.27
	assign (segid 3A4 and resid 137 and name N)	(segid 3A4 and resid 138 and name N)	2.24	0.01	0.01
70	assign (segid 3A4 and resid 137 and name N)	(segid 3A4 and resid 138 and name O)	4.23	0.41	0.41
	assign (segid 3A4 and resid 137 and name N)	(segid 3A4 and resid 139 and name C)	6.29	0.32	0.31
	assign (segid 3A4 and resid 137 and name N)	(segid 3A4 and resid 139 and name CA)	5.05	0.41	0.41
	assign (segid 3A4 and resid 137 and name N)	(segid 3A4 and resid 139 and name N)	3.87	0.31	0.31
75	assign (segid 3A4 and resid 137 and name N)	(segid 3A4 and resid 140 and name CA)	7.81	0.11	0.11
	assign (segid 3A4 and resid 137 and name N)	(segid 3A4 and resid 140 and name N)	6.47	0.17	0.17
	assign (segid 3A4 and resid 137 and name N)	(segid 3A4 and resid 219 and name C)	3.98	0.35	0.35
	assign (segid 3A4 and resid 137 and name N)	(segid 3A4 and resid 219 and name CA)	4.01	0.50	0.50
	assign (segid 3A4 and resid 137 and name N)	(segid 3A4 and resid 219 and name CB)	3.68	0.22	0.21
80	assign (segid 3A4 and resid 137 and name N)	(segid 3A4 and resid 219 and name CG)	4.42	0.43	0.44
	assign (segid 3A4 and resid 137 and name N)	(segid 3A4 and resid 219 and name N)	5.34	0.41	0.40
	assign (segid 3A4 and resid 137 and name N)	(segid 3A4 and resid 219 and name O)	5.01	0.12	0.12
	assign (segid 3A4 and resid 137 and name N)	(segid 3A4 and resid 220 and name C)	4.70	0.37	0.37

5	assign (segid 3A4 and resid 137 and name O)	(segid 3A4 and resid 220 and name CA)	4.01	0.31	0.32
	assign (segid 3A4 and resid 137 and name O)	(segid 3A4 and resid 220 and name CB)	3.81	0.27	0.28
	assign (segid 3A4 and resid 137 and name O)	(segid 3A4 and resid 220 and name N)	3.27	0.50	0.49
	assign (segid 3A4 and resid 137 and name O)	(segid 3A4 and resid 220 and name O)	5.86	0.37	0.36
	assign (segid 3A4 and resid 137 and name O)	(segid 3A4 and resid 221 and name C)	6.51	0.74	0.73
	assign (segid 3A4 and resid 137 and name O)	(segid 3A4 and resid 221 and name CA)	5.48	0.84	0.84
	assign (segid 3A4 and resid 137 and name O)	(segid 3A4 and resid 221 and name CB)	5.44	1.08	1.07
	assign (segid 3A4 and resid 137 and name O)	(segid 3A4 and resid 221 and name N)	4.34	0.63	0.64
	assign (segid 3A4 and resid 137 and name O)	(segid 3A4 and resid 222 and name CB)	7.64	0.29	0.30
10	assign (segid 3A4 and resid 137 and name O)	(segid 3A4 and resid 222 and name N)	6.38	0.58	0.58
	assign (segid 3A4 and resid 137 and name O)	(segid 3A4 and resid 223 and name N)	7.64	0.23	0.23
	assign (segid 3A4 and resid 138 and name C)	(segid 3A4 and resid 138 and name CB)	2.48	0.02	0.03
	assign (segid 3A4 and resid 138 and name C)	(segid 3A4 and resid 138 and name O)	1.24	0.01	0.00
	assign (segid 3A4 and resid 138 and name C)	(segid 3A4 and resid 139 and name C)	3.28	0.16	0.17
15	assign (segid 3A4 and resid 138 and name C)	(segid 3A4 and resid 139 and name CA)	2.44	0.01	0.02
	assign (segid 3A4 and resid 138 and name C)	(segid 3A4 and resid 139 and name N)	1.33	0.01	0.01
	assign (segid 3A4 and resid 138 and name C)	(segid 3A4 and resid 139 and name O)	4.27	0.24	0.24
	assign (segid 3A4 and resid 138 and name C)	(segid 3A4 and resid 140 and name C)	5.82	0.26	0.26
	assign (segid 3A4 and resid 138 and name C)	(segid 3A4 and resid 140 and name CA)	4.78	0.26	0.25
20	assign (segid 3A4 and resid 138 and name C)	(segid 3A4 and resid 140 and name CB)	5.09	0.37	0.37
	assign (segid 3A4 and resid 138 and name C)	(segid 3A4 and resid 140 and name N)	3.48	0.20	0.19
	assign (segid 3A4 and resid 138 and name C)	(segid 3A4 and resid 140 and name O)	5.84	0.34	0.35
	assign (segid 3A4 and resid 138 and name C)	(segid 3A4 and resid 141 and name N)	6.95	0.22	0.22
	assign (segid 3A4 and resid 138 and name C)	(segid 3A4 and resid 219 and name C)	5.57	0.64	0.63
25	assign (segid 3A4 and resid 138 and name C)	(segid 3A4 and resid 219 and name CA)	5.28	0.46	0.46
	assign (segid 3A4 and resid 138 and name C)	(segid 3A4 and resid 219 and name CB)	4.08	0.29	0.28
	assign (segid 3A4 and resid 138 and name C)	(segid 3A4 and resid 219 and name CG)	4.19	0.11	0.10
	assign (segid 3A4 and resid 138 and name C)	(segid 3A4 and resid 219 and name N)	6.35	0.25	0.25
	assign (segid 3A4 and resid 138 and name C)	(segid 3A4 and resid 219 and name O)	6.45	0.55	0.54
30	assign (segid 3A4 and resid 138 and name C)	(segid 3A4 and resid 220 and name C)	6.09	0.87	0.88
	assign (segid 3A4 and resid 138 and name C)	(segid 3A4 and resid 220 and name CA)	6.00	0.95	0.95
	assign (segid 3A4 and resid 138 and name C)	(segid 3A4 and resid 220 and name CB)	6.02	1.01	1.02
	assign (segid 3A4 and resid 138 and name C)	(segid 3A4 and resid 220 and name N)	5.21	0.89	0.89
	assign (segid 3A4 and resid 138 and name C)	(segid 3A4 and resid 221 and name CA)	5.79	0.71	0.71
35	assign (segid 3A4 and resid 138 and name C)	(segid 3A4 and resid 221 and name CB)	5.03	0.60	0.61
	assign (segid 3A4 and resid 138 and name C)	(segid 3A4 and resid 221 and name N)	5.19	0.84	0.83
	assign (segid 3A4 and resid 138 and name C)	(segid 3A4 and resid 222 and name N)	6.64	0.42	0.43
	assign (segid 3A4 and resid 138 and name CA)	(segid 3A4 and resid 138 and name C)	1.53	0.01	0.00
	assign (segid 3A4 and resid 138 and name CA)	(segid 3A4 and resid 138 and name CB)	1.52	0.01	0.01
40	assign (segid 3A4 and resid 138 and name CA)	(segid 3A4 and resid 138 and name O)	2.40	0.02	0.02
	assign (segid 3A4 and resid 138 and name CA)	(segid 3A4 and resid 139 and name C)	4.59	0.12	0.12
	assign (segid 3A4 and resid 138 and name CA)	(segid 3A4 and resid 139 and name CA)	3.80	0.02	0.03
	assign (segid 3A4 and resid 138 and name CA)	(segid 3A4 and resid 139 and name N)	2.42	0.02	0.03
	assign (segid 3A4 and resid 138 and name CA)	(segid 3A4 and resid 139 and name O)	5.66	0.20	0.19
45	assign (segid 3A4 and resid 138 and name CA)	(segid 3A4 and resid 140 and name C)	6.66	0.34	0.33
	assign (segid 3A4 and resid 138 and name CA)	(segid 3A4 and resid 140 and name CA)	5.68	0.21	0.21
	assign (segid 3				

	assign (segid 3A4 and resid 138 and name CA)	(segid 3A4 and resid 202 and name CA)	9.82	0.97	0.96
	assign (segid 3A4 and resid 138 and name CA)	(segid 3A4 and resid 202 and name CB)	10.43	0.89	0.88
	assign (segid 3A4 and resid 138 and name CA)	(segid 3A4 and resid 203 and name CA)	13.09	1.04	1.05
	assign (segid 3A4 and resid 138 and name CA)	(segid 3A4 and resid 203 and name CB)	14.09	1.06	1.07
5	assign (segid 3A4 and resid 138 and name CA)	(segid 3A4 and resid 204 and name CA)	12.13	1.05	1.06
	assign (segid 3A4 and resid 138 and name CA)	(segid 3A4 and resid 204 and name CB)	11.56	0.97	0.98
	assign (segid 3A4 and resid 138 and name CA)	(segid 3A4 and resid 205 and name CA)	10.03	1.01	1.01
	assign (segid 3A4 and resid 138 and name CA)	(segid 3A4 and resid 205 and name CB)	8.75	0.91	0.91
	assign (segid 3A4 and resid 138 and name CA)	(segid 3A4 and resid 206 and name CA)	13.17	0.89	0.89
10	assign (segid 3A4 and resid 138 and name CA)	(segid 3A4 and resid 206 and name CB)	13.90	0.86	0.86
	assign (segid 3A4 and resid 138 and name CA)	(segid 3A4 and resid 207 and name CA)	15.34	1.00	1.00
	assign (segid 3A4 and resid 138 and name CA)	(segid 3A4 and resid 207 and name CB)	15.78	1.09	1.09
	assign (segid 3A4 and resid 138 and name CA)	(segid 3A4 and resid 219 and name C)	5.62	0.44	0.44
	assign (segid 3A4 and resid 138 and name CA)	(segid 3A4 and resid 219 and name CA)	5.61	0.32	0.31
15	assign (segid 3A4 and resid 138 and name CA)	(segid 3A4 and resid 219 and name CB)	4.66	0.16	0.16
	assign (segid 3A4 and resid 138 and name CA)	(segid 3A4 and resid 219 and name CG)	4.93	0.44	0.44
	assign (segid 3A4 and resid 138 and name CA)	(segid 3A4 and resid 219 and name N)	6.84	0.16	0.15
	assign (segid 3A4 and resid 138 and name CA)	(segid 3A4 and resid 219 and name O)	6.54	0.30	0.29
	assign (segid 3A4 and resid 138 and name CA)	(segid 3A4 and resid 220 and name C)	5.71	0.65	0.65
20	assign (segid 3A4 and resid 138 and name CA)	(segid 3A4 and resid 220 and name CA)	5.51	0.80	0.80
	assign (segid 3A4 and resid 138 and name CA)	(segid 3A4 and resid 220 and name CB)	5.17	0.93	0.94
	assign (segid 3A4 and resid 138 and name CA)	(segid 3A4 and resid 220 and name N)	4.96	0.73	0.73
	assign (segid 3A4 and resid 138 and name CA)	(segid 3A4 and resid 221 and name C)	6.86	0.35	0.35
	assign (segid 3A4 and resid 138 and name CA)	(segid 3A4 and resid 221 and name CA)	5.67	0.42	0.42
25	assign (segid 3A4 and resid 138 and name CA)	(segid 3A4 and resid 221 and name CB)	5.08	0.41	0.41
	assign (segid 3A4 and resid 138 and name CA)	(segid 3A4 and resid 221 and name N)	4.95	0.52	0.53
	assign (segid 3A4 and resid 138 and name CA)	(segid 3A4 and resid 222 and name CA)	8.21	0.19	0.19
	assign (segid 3A4 and resid 138 and name CA)	(segid 3A4 and resid 222 and name CB)	8.38	0.14	0.14
	assign (segid 3A4 and resid 138 and name CA)	(segid 3A4 and resid 222 and name N)	6.91	0.22	0.21
30	assign (segid 3A4 and resid 138 and name CA)	(segid 3A4 and resid 223 and name CA)	9.84	0.43	0.43
	assign (segid 3A4 and resid 138 and name CA)	(segid 3A4 and resid 223 and name CB)	9.61	0.61	0.60
	assign (segid 3A4 and resid 138 and name CA)	(segid 3A4 and resid 224 and name CA)	10.32	0.54	0.54
	assign (segid 3A4 and resid 138 and name CA)	(segid 3A4 and resid 224 and name CB)	9.56	0.54	0.53
	assign (segid 3A4 and resid 138 and name CA)	(segid 3A4 and resid 225 and name CA)	11.56	0.35	0.34
35	assign (segid 3A4 and resid 138 and name CA)	(segid 3A4 and resid 225 and name CB)	11.01	0.31	0.32
	assign (segid 3A4 and resid 138 and name CA)	(segid 3A4 and resid 226 and name CA)	13.95	0.32	0.31
	assign (segid 3A4 and resid 138 and name CA)	(segid 3A4 and resid 240 and name CA)	17.51	0.68	0.68
	assign (segid 3A4 and resid 138 and name CA)	(segid 3A4 and resid 240 and name CB)	18.62	0.66	0.67
	assign (segid 3A4 and resid 138 and name CA)	(segid 3A4 and resid 241 and name CA)	15.38	0.89	0.88
40	assign (segid 3A4 and resid 138 and name CA)	(segid 3A4 and resid 241 and name CB)	15.97	1.03	1.03
	assign (segid 3A4 and resid 138 and name CA)	(segid 3A4 and resid 242 and name CA)	16.29	0.84	0.84
	assign (segid 3A4 and resid 138 and name CA)	(segid 3A4 and resid 242 and name CB)	17.74	0.85	0.85
	assign (segid 3A4 and resid 138 and name CA)	(segid 3A4 and resid 243 and name CA)	15.39	0.77	0.76
	assign (segid 3A4 and resid 138 and name CA)	(segid 3A4 and resid 243 and name CB)	16.09	0.71	0.72
45	assign (segid 3A4 and resid 138 and name CA)	(segid 3A4 and resid 244 and name CA)	11.94	0.74	0.74
	assign (segid 3A4 and resid 138 and name CA)	(segid 3A4 and resid 244 and name CB)	11.74	0.74	0.74
	assign (segid 3A4 and resid 138 and name CA)	(segid 3A4 and resid 245 and name CA)	11.65	0.83	0.82
	assign (segid 3A4 and resid 138 and name CA)	(segid 3A4 and resid 245 and name CB)	12.72	0.85	0.85
	assign (segid 3A4 and resid 138 and name CA)	(segid 3A4 and resid 246 and name CA)	13.42	0.81	0.80
50	assign (segid 3A4 and resid 138 and name CA)	(segid 3A4 and resid 246 and name CB)	14.81	0.83	0.83
	assign (segid 3A4 and resid 138 and name CA)	(segid 3A4 and resid 247 and name CA)	11.38	0.88	0.87
	assign (segid 3A4 and resid 138 and name CA)	(segid 3A4 and resid 247 and name CB)	11.24	0.82	0.83
	assign (segid 3A4 and resid 138 and name CA)	(segid 3A4 and resid 248 and name CA)	8.18	0.83	0.83
	assign (segid 3A4 and resid 138 and name CA)	(segid 3A4 and resid 248 and name CB)	7.68	0.74	0.74
55	assign (segid 3A4 and resid 138 and name CA)	(segid 3A4 and resid 249 and name CA)	10.71	0.87	0.87
	assign (segid 3A4 and resid 138 and name CA)	(segid 3A4 and resid 250 and name CA)	12.17	1.08	1.09
	assign (segid 3A4 and resid 138 and name CA)	(segid 3A4 and resid 250 and name CB)	12.90	1.12	1.12
	assign (segid 3A4 and resid 138 and name CA)	(segid 3A4 and resid 251 and name CA)	9.45	1.25	1.25
	assign (segid 3A4 and resid 138 and name CA)	(segid 3A4 and resid 251 and name CB)	8.29	1.21	1.22
60	assign (segid 3A4 and resid 138 and name CA)	(segid 3A4 and resid 252 and name CA)	9.11	1.24	1.25
	assign (segid 3A4 and resid 138 and name CA)	(segid 3A4 and resid 252 and name CB)	8.93	1.11	1.11
	assign (segid 3A4 and resid 138 and name CA)	(segid 3A4 and resid 253 and name CA)	12.83	1.20	1.21
	assign (segid 3A4 and resid 138 and name CA)	(segid 3A4 and resid 254 and name CA)	13.86	1.46	1.47
	assign (segid 3A4 and resid 138 and name CA)	(segid 3A4 and resid 255 and name CA)	12.19	1.75	1.75
65	assign (segid 3A4 and resid 138 and name CA)	(segid 3A4 and resid 256 and name CA)	13.06	1.07	1.07
	assign (segid 3A4 and resid 138 and name CA)	(segid 3A4 and resid 257 and name CA)	16.66	1.19	1.18
	assign (segid 3A4 and resid 138 and name CA)	(segid 3A4 and resid 259 and name CA)	17.00	1.00	0.99
	assign (segid 3A4 and resid 138 and name CA)	(segid 3A4 and resid 259 and name CB)	15.69	0.95	0.96
	assign (segid 3A4 and resid 138 and name CA)	(segid 3A4 and resid 260 and name CA)	18.21	0.88	0.87
70	assign (segid 3A4 and resid 138 and name CA)	(segid 3A4 and resid 260 and name CB)	17.84	0.86	0.86
	assign (segid 3A4 and resid 138 and name CA)	(segid 3A4 and resid 392 and name CA)	15.78	1.20	1.20
	assign (segid 3A4 and resid 138 and name CA)	(segid 3A4 and resid 392 and name CB)	14.92	1.21	1.21
	assign (segid 3A4 and resid 138 and name CA)	(segid 3A4 and resid 393 and name CA)	14.05	1.15	1.15
	assign (segid 3A4 and resid 138 and name CA)	(segid 3A4 and resid 394 and name CA)	17.50	1.15	1.14
75	assign (segid 3A4 and resid 138 and name CA)	(segid 3A4 and resid 395 and name CA)	17.06	1.01	1.00
	assign (segid 3A4 and resid 138 and name CA)	(segid 3A4 and resid 396 and name CA)	14.00	1.01	1.01
	assign (segid 3A4 and resid 138 and name CA)	(segid 3A4 and resid 396 and name CB)	12.56	1.02	1.02
	assign (segid 3A4 and resid 138 and name CA)	(segid 3A4 and resid 397 and name CA)	15.93	0.96	0.95
	assign (segid 3A4 and resid 138 and name CA)	(segid 3A4 and resid 397 and name CB)	16.50	0.97	0.97
80	assign (segid 3A4 and resid 138 and name CA)	(segid 3A4 and resid 399 and name CA)	17.73	0.85	0.84
	assign (segid 3A4 and resid 138 and name CA)	(segid 3A4 and resid 399 and name CB)	16.72	0.83	0.83
	assign (segid 3A4 and resid 138 and name CA)	(segid 3A4 and resid 400 and name CA)	16.38	0.79	0.79
	assign (segid 3A4 and resid 138 and name CA)	(segid 3A4 and resid 400 and name CB)	15.32	0.89	0.88

	assign (segid 3A4 and resid 138 and name CA)	(segid 3A4 and resid 403 and name CB)	19.01	0.55	0.56
	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 139 and name C)	4.96	0.19	0.20
	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 139 and name CA)	4.60	0.15	0.15
	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 139 and name N)	3.32	0.15	0.16
5	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 139 and name O)	6.01	0.21	0.21
	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 140 and name C)	6.46	0.55	0.55
	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 140 and name CB)	5.42	0.34	0.33
	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 140 and name N)	5.07	0.36	0.35
	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 140 and name O)	4.52	0.31	0.30
10	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 141 and name CA)	6.40	0.68	0.68
	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 141 and name CB)	8.81	0.66	0.67
	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 141 and name CB)	9.88	0.62	0.63
	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 147 and name CA)	12.73	1.87	1.86
	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 147 and name CB)	13.68	1.77	1.77
	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 148 and name CA)	13.21	0.44	0.43
15	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 149 and name CA)	11.79	0.75	0.75
	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 149 and name CB)	11.13	1.07	1.07
	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 150 and name CA)	12.70	2.06	2.06
	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 151 and name CA)	14.77	0.80	0.81
	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 152 and name CA)	13.91	0.83	0.82
20	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 152 and name CB)	13.41	1.13	1.13
	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 153 and name CA)	12.91	2.10	2.10
	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 153 and name CB)	12.13	2.68	2.69
	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 155 and name CA)	16.78	1.18	1.18
	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 155 and name CB)	16.89	0.90	0.91
25	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 156 and name CA)	15.80	1.70	1.71
	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 156 and name CB)	14.83	1.82	1.81
	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 190 and name CA)	18.35	0.77	0.77
	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 190 and name CB)	18.56	0.79	0.79
	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 191 and name CA)	16.90	0.76	0.75
30	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 191 and name CB)	17.75	0.78	0.79
	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 192 and name CA)	17.46	0.75	0.76
	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 192 and name CB)	18.87	0.76	0.76
	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 193 and name CA)	15.84	0.78	0.78
	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 193 and name CB)	16.32	0.82	0.82
35	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 194 and name CA)	12.58	0.70	0.69
	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 194 and name CB)	12.51	0.70	0.71
	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 195 and name CA)	13.11	0.77	0.78
	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 195 and name CB)	14.37	0.76	0.76
40	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 196 and name CA)	14.04	0.97	0.97
	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 196 and name CB)	15.17	1.00	1.00
	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 197 and name CA)	11.13	0.93	0.93
	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 197 and name CB)	10.79	0.82	0.81
	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 198 and name CA)	8.85	0.92	0.92
	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 198 and name CB)	8.84	0.83	0.82
45	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 199 and name CA)	11.65	1.10	1.11
	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 199 and name CB)	13.07	1.08	1.08
	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 200 and name CA)	11.86	1.26	1.26
	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 201 and name CA)	8.48	1.29	1.30
	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 201 and name CB)	7.12	1.30	1.30
50	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 202 and name CA)	9.55	1.09	1.09
	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 202 and name CB)	10.06	1.03	1.03
	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 203 and name CA)	12.89	1.19	1.18
	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 203 and name CB)	13.77	1.22	1.22
	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 204 and name CA)	12.13	1.21	1.21
55	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 204 and name CB)	11.50	1.16	1.15
	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 205 and name CA)	10.39	1.10	1.09
	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 205 and name CB)	9.11	0.98	0.98
	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 206 and name CA)	13.51	0.98	0.99
	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 206 and name CB)	14.11	0.97	0.97
60	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 207 and name CA)	15.71	1.12	1.12
	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 207 and name CB)	16.05	1.24	1.23
	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 219 and name CA)	7.05	0.33	0.33
	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 219 and name CB)	6.07	0.18	0.19
	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 219 and name CG)	6.19	0.39	0.39
65	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 220 and name CA)	6.55	0.84	0.84
	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 220 and name CB)	6.04	0.97	0.97
	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 221 and name CA)	6.22	0.66	0.67
	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 221 and name CB)	5.44	0.65	0.65
	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 221 and name N)	5.75	0.69	0.68
70	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 222 and name CA)	9.12	0.37	0.37
	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 222 and name CB)	9.43	0.21	0.22
	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 223 and name CA)	10.82	0.56	0.57
	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 223 and name CB)	10.64	0.68	0.68
	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 224 and name CA)	10.83	0.79	0.80
75	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 224 and name CB)	9.91	0.81	0.81
	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 225 and name CA)	11.99	0.63	0.62
	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 225 and name CB)	11.45	0.57	0.57
	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 226 and name CA)	14.66	0.54	0.55
	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 240 and name CA)	17.32	0.88	0.88
80	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 240 and name CB)	18.36	0.88	0.88
	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 241 and name CA)	15.02	1.05	1.06
	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 241 and name CB)	15.58	1.19	1.19

	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 242 and name CA)	15.69	1.03	1.03
	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 242 and name CB)	17.11	1.03	1.04
	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 243 and name CA)	14.94	1.05	1.05
	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 243 and name CB)	15.76	1.01	1.01
5	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 244 and name CA)	11.62	1.00	1.00
	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 244 and name CB)	11.51	0.97	0.96
	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 245 and name CA)	10.92	1.04	1.04
	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 245 and name CB)	11.93	1.05	1.05
	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 246 and name CA)	12.63	1.07	1.07
10	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 246 and name CB)	14.06	1.10	1.10
	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 247 and name CA)	10.85	1.15	1.16
	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 247 and name CB)	10.89	1.10	1.11
	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 248 and name CA)	7.46	1.11	1.12
	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 248 and name CB)	6.94	1.01	1.01
15	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 249 and name CA)	9.66	1.15	1.15
	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 250 and name CA)	11.33	1.40	1.40
	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 250 and name CB)	12.16	1.42	1.43
	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 251 and name CA)	8.83	1.58	1.58
	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 251 and name CB)	7.82	1.52	1.52
20	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 252 and name CA)	8.12	1.60	1.60
	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 252 and name CB)	7.82	1.44	1.43
	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 253 and name CA)	11.80	1.52	1.52
	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 254 and name CA)	13.10	1.77	1.77
	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 255 and name CA)	11.59	2.03	2.03
25	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 256 and name CA)	12.29	1.38	1.39
	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 257 and name CA)	15.82	1.50	1.49
	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 259 and name CA)	16.57	1.26	1.25
	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 259 and name CB)	15.33	1.20	1.20
	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 260 and name CA)	17.62	1.15	1.15
30	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 260 and name CB)	17.16	1.13	1.14
	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 392 and name CA)	15.88	1.37	1.37
	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 392 and name CB)	15.00	1.38	1.38
	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 393 and name CA)	14.14	1.33	1.34
	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 395 and name CA)	17.49	1.16	1.15
35	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 396 and name CA)	14.38	1.14	1.14
	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 396 and name CB)	12.92	1.16	1.15
	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 397 and name CA)	16.00	1.12	1.12
	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 397 and name CB)	16.49	1.16	1.16
	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 399 and name CA)	18.15	0.95	0.95
40	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 399 and name CB)	17.24	0.93	0.92
	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 400 and name CA)	16.60	0.87	0.87
	assign (segid 3A4 and resid 138 and name CB)	(segid 3A4 and resid 400 and name CB)	15.46	0.97	0.96
	assign (segid 3A4 and resid 138 and name N)	(segid 3A4 and resid 138 and name C)	2.48	0.03	0.04
45	assign (segid 3A4 and resid 138 and name N)	(segid 3A4 and resid 138 and name CB)	1.46	0.01	0.00
	assign (segid 3A4 and resid 138 and name N)	(segid 3A4 and resid 138 and name O)	3.58	0.05	0.05
	assign (segid 3A4 and resid 138 and name N)	(segid 3A4 and resid 139 and name C)	5.07	0.09	0.09
	assign (segid 3A4 and resid 138 and name N)	(segid 3A4 and resid 139 and name CA)	4.18	0.06	0.06
50	assign (segid 3A4 and resid 138 and name N)	(segid 3A4 and resid 139 and name O)	2.76	0.06	0.06
	assign (segid 3A4 and resid 138 and name N)	(segid 3A4 and resid 140 and name C)	6.84	0.29	0.29
	assign (segid 3A4 and resid 138 and name N)	(segid 3A4 and resid 140 and name CA)	6.12	0.14	0.15
	assign (segid 3A4 and resid 138 and name N)	(segid 3A4 and resid 140 and name CB)	6.17	0.20	0.21
	assign (segid 3A4 and resid 138 and name N)	(segid 3A4 and resid 140 and name O)	4.90	0.12	0.11
55	assign (segid 3A4 and resid 138 and name N)	(segid 3A4 and resid 140 and name O)	6.45	0.42	0.42
	assign (segid 3A4 and resid 138 and name N)	(segid 3A4 and resid 219 and name C)	5.68	0.14	0.14
	assign (segid 3A4 and resid 138 and name N)	(segid 3A4 and resid 219 and name CA)	5.54	0.12	0.12
	assign (segid 3A4 and resid 138 and name N)	(segid 3A4 and resid 219 and name CB)	4.75	0.23	0.23
	assign (segid 3A4 and resid 138 and name N)	(segid 3A4 and resid 219 and name CG)	5.38	0.62	0.61
60	assign (segid 3A4 and resid 138 and name N)	(segid 3A4 and resid 219 and name N)	6.85	0.10	0.09
	assign (segid 3A4 and resid 138 and name N)	(segid 3A4 and resid 219 and name O)	6.74	0.07	0.06
	assign (segid 3A4 and resid 138 and name N)	(segid 3A4 and resid 220 and name C)	6.13	0.22	0.22
	assign (segid 3A4 and resid 138 and name N)	(segid 3A4 and resid 220 and name CA)	5.60	0.37	0.36
	assign (segid 3A4 and resid 138 and name N)	(segid 3A4 and resid 220 and name CB)	5.11	0.47	0.46
65	assign (segid 3A4 and resid 138 and name N)	(segid 3A4 and resid 220 and name N)	4.94	0.34	0.35
	assign (segid 3A4 and resid 138 and name N)	(segid 3A4 and resid 220 and name O)	7.29	0.23	0.24
	assign (segid 3A4 and resid 138 and name N)	(segid 3A4 and resid 221 and name CA)	6.51	0.34	0.34
	assign (segid 3A4 and resid 138 and name N)	(segid 3A4 and resid 221 and name CB)	6.11	0.51	0.51
	assign (segid 3A4 and resid 138 and name N)	(segid 3A4 and resid 221 and name N)	5.58	0.23	0.23
70	assign (segid 3A4 and resid 138 and name O)	(segid 3A4 and resid 138 and name CB)	3.08	0.14	0.13
	assign (segid 3A4 and resid 138 and name O)	(segid 3A4 and resid 139 and name C)	3.45	0.33	0.32
	assign (segid 3A4 and resid 138 and name O)	(segid 3A4 and resid 139 and name N)	2.25	0.00	0.01
	assign (segid 3A4 and resid 138 and name O)	(segid 3A4 and resid 139 and name O)	4.17	0.46	0.46
75	assign (segid 3A4 and resid 138 and name O)	(segid 3A4 and resid 140 and name C)	6.17	0.43	0.42
	assign (segid 3A4 and resid 138 and name O)	(segid 3A4 and resid 140 and name CA)	4.97	0.51	0.51
	assign (segid 3A4 and resid 138 and name O)	(segid 3A4 and resid 140 and name CB)	5.28	0.71	0.70
	assign (segid 3A4 and resid 138 and name O)	(segid 3A4 and resid 140 and name N)	3.81	0.37	0.38
	assign (segid 3A4 and resid 138 and name O)	(segid 3A4 and resid 140 and name O)	6.40	0.42	0.42
80	assign (segid 3A4 and resid 138 and name O)	(segid 3A4 and resid 141 and name N)	7.18	0.40	0.39
	assign (segid 3A4 and resid 138 and name O)	(segid 3A4 and resid 201 and name CB)	6.58	0.55	0.56
	assign (segid 3A4 and resid 138 and name O)	(segid 3A4 and resid 205 and name CB)	7.05	0.51	0.51
	assign (segid 3A4 and resid 138 and name O)	(segid 3A4 and resid 219 and name C)	5.61	1.01	1.01

	assign (segid 3A4 and resid 138 and name O)	(segid 3A4 and resid 219 and name CA)	5.44	0.76	0.75
	assign (segid 3A4 and resid 138 and name O)	(segid 3A4 and resid 219 and name CB)	4.21	0.58	0.59
	assign (segid 3A4 and resid 138 and name O)	(segid 3A4 and resid 219 and name CG)	3.97	0.38	0.39
	assign (segid 3A4 and resid 138 and name O)	(segid 3A4 and resid 219 and name N)	6.38	0.56	0.56
5	assign (segid 3A4 and resid 138 and name O)	(segid 3A4 and resid 220 and name N)	5.39	1.25	1.26
	assign (segid 3A4 and resid 138 and name O)	(segid 3A4 and resid 221 and name C)	6.18	0.95	0.96
	assign (segid 3A4 and resid 138 and name O)	(segid 3A4 and resid 221 and name CA)	5.27	1.14	1.14
	assign (segid 3A4 and resid 138 and name O)	(segid 3A4 and resid 221 and name CB)	4.38	0.98	0.99
	assign (segid 3A4 and resid 138 and name O)	(segid 3A4 and resid 221 and name N)	4.88	1.30	1.30
10	assign (segid 3A4 and resid 138 and name O)	(segid 3A4 and resid 222 and name N)	6.05	0.84	0.83
	assign (segid 3A4 and resid 139 and name C)	(segid 3A4 and resid 139 and name O)	1.24	0.02	0.01
	assign (segid 3A4 and resid 139 and name C)	(segid 3A4 and resid 140 and name CA)	3.27	0.12	0.12
	assign (segid 3A4 and resid 139 and name C)	(segid 3A4 and resid 140 and name CB)	2.45	0.03	0.03
	assign (segid 3A4 and resid 139 and name C)	(segid 3A4 and resid 140 and name N)	3.62	0.09	0.10
15	assign (segid 3A4 and resid 139 and name C)	(segid 3A4 and resid 140 and name O)	1.32	0.01	0.01
	assign (segid 3A4 and resid 139 and name C)	(segid 3A4 and resid 140 and name O)	3.65	0.13	0.13
	assign (segid 3A4 and resid 139 and name C)	(segid 3A4 and resid 141 and name C)	6.38	0.24	0.24
	assign (segid 3A4 and resid 139 and name C)	(segid 3A4 and resid 141 and name CA)	5.32	0.24	0.25
	assign (segid 3A4 and resid 139 and name C)	(segid 3A4 and resid 141 and name CB)	6.04	0.27	0.26
20	assign (segid 3A4 and resid 139 and name C)	(segid 3A4 and resid 141 and name N)	4.15	0.22	0.22
	assign (segid 3A4 and resid 139 and name C)	(segid 3A4 and resid 141 and name O)	6.68	0.29	0.29
	assign (segid 3A4 and resid 139 and name C)	(segid 3A4 and resid 219 and name CA)	7.05	0.39	0.40
	assign (segid 3A4 and resid 139 and name C)	(segid 3A4 and resid 219 and name CB)	5.61	0.41	0.40
	assign (segid 3A4 and resid 139 and name C)	(segid 3A4 and resid 219 and name CG)	5.56	0.41	0.41
25	assign (segid 3A4 and resid 139 and name C)	(segid 3A4 and resid 139 and name C)	1.51	0.01	0.02
	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 139 and name O)	2.39	0.02	0.01
	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 140 and name C)	4.56	0.07	0.08
	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 140 and name CA)	3.82	0.04	0.04
	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 140 and name CB)	4.80	0.09	0.09
30	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 140 and name N)	2.44	0.03	0.03
	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 140 and name O)	4.65	0.11	0.11
	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 141 and name CA)	6.58	0.22	0.22
	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 141 and name CB)	7.32	0.28	0.28
	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 141 and name N)	5.52	0.19	0.20
35	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 147 and name CA)	12.14	3.25	3.25
	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 147 and name CB)	12.94	3.23	3.23
	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 148 and name CA)	12.96	1.44	1.43
	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 149 and name CA)	12.13	1.55	1.55
	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 149 and name CB)	11.28	1.80	1.80
40	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 150 and name CA)	13.65	2.76	2.75
	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 151 and name CA)	16.24	1.65	1.64
	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 152 and name CA)	15.65	0.97	0.97
	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 152 and name CB)	14.93	0.78	0.79
	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 193 and name CB)	18.33	0.87	0.88
45	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 193 and name CB)	18.76	0.88	0.87
	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 194 and name CA)	15.45	0.94	0.95
	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 194 and name CB)	15.67	1.01	1.01
	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 195 and name CA)	16.05	0.94	0.95
	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 195 and name CB)	17.41	0.96	0.96
50	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 196 and name CA)	16.20	0.73	0.73
	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 196 and name CB)	17.21	0.71	0.70
	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 197 and name CA)	12.94	0.72	0.71
	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 197 and name CB)	12.69	0.76	0.77
	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 198 and name CA)	11.19	0.81	0.81
	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 198 and name CB)	11.62	0.87	0.88
55	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 199 and name CA)	13.54	0.73	0.73
	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 199 and name CB)	15.02	0.74	0.75
	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 200 and name CA)	12.68	0.69	0.69
	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 201 and name CA)	9.02	0.69	0.68
	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 201 and name CB)	8.03	0.66	0.65
60	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 202 and name CA)	10.59	0.67	0.67
	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 202 and name CB)	11.59	0.66	0.65
	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 203 and name CA)	13.19	0.70	0.71
	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 203 and name CB)	14.14	0.68	0.68
65	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 204 and name CA)	11.30	0.69	0.69
	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 204 and name CB)	10.49	0.67	0.68
	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 205 and name CA)	9.50	0.71	0.71
	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 205 and name CB)	8.57	0.69	0.69
	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 206 and name CA)	13.06	0.68	0.68
	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 206 and name CB)	14.02	0.68	0.67
70	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 207 and name CA)	14.45	0.77	0.76
	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 207 and name CB)	14.76	0.74	0.74
	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 219 and name C)	6.43	0.49	0.49
	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 219 and name CA)	5.62	0.35	0.35
75	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 219 and name CB)	4.20	0.35	0.35
	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 219 and name N)	4.33	0.38	0.37
	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 220 and name CA)	7.56	0.69	0.69
	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 220 and name CB)	7.82	0.67	0.68
	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 220 and name N)	6.46	0.63	0.63
80	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 221 and name CA)	7.39	0.86	0.86
	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 221 and name CB)	6.56	0.90	0.91
	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 222 and name CA)	8.63	0.60	0.60

	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 222 and name CB)	8.25	0.54	0.53
	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 223 and name CA)	11.03	0.61	0.62
	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 223 and name CB)	11.00	0.66	0.65
	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 224 and name CA)	12.30	0.75	0.75
5	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 224 and name CB)	11.85	0.75	0.75
	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 225 and name CA)	12.80	0.74	0.75
	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 225 and name CB)	11.93	0.70	0.70
	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 226 and name CA)	14.81	0.68	0.67
	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 241 and name CA)	17.25	0.72	0.72
10	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 241 and name CB)	17.63	0.84	0.84
	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 242 and name CA)	18.59	0.88	0.88
	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 243 and name CA)	18.07	0.90	0.90
	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 244 and name CA)	14.44	0.86	0.85
	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 244 and name CB)	13.98	0.80	0.80
15	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 245 and name CA)	14.07	0.91	0.91
	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 245 and name CB)	14.97	0.93	0.93
	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 246 and name CA)	16.31	0.96	0.96
	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 246 and name CB)	17.73	0.96	0.97
	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 247 and name CA)	14.54	0.85	0.85
20	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 247 and name CB)	14.36	0.78	0.79
	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 248 and name CA)	11.19	0.90	0.89
	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 248 and name CB)	10.44	0.89	0.88
	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 249 and name CA)	13.55	1.01	1.02
	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 250 and name CA)	15.39	0.94	0.94
25	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 250 and name CB)	16.19	0.94	0.95
	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 251 and name CA)	12.71	0.82	0.83
	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 251 and name CB)	11.59	0.76	0.76
	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 252 and name CA)	11.88	0.99	1.00
	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 252 and name CB)	11.52	1.05	1.05
30	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 253 and name CA)	15.59	1.02	1.03
	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 254 and name CA)	16.87	1.00	1.00
	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 255 and name CA)	14.90	1.39	1.39
	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 256 and name CA)	15.24	0.69	0.69
	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 257 and name CA)	18.86	0.76	0.76
35	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 259 and name CA)	19.01	0.26	0.25
	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 259 and name CB)	17.66	0.23	0.22
	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 392 and name CA)	18.83	0.58	0.57
	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 392 and name CB)	18.07	0.64	0.63
	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 393 and name CA)	16.85	0.43	0.43
40	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 395 and name CA)	19.19	0.49	0.48
	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 396 and name CA)	15.95	0.48	0.48
	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 396 and name CB)	14.65	0.50	0.49
	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 397 and name CA)	18.00	0.46	0.46
	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 397 and name CB)	18.77	0.40	0.40
45	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 399 and name CA)	19.00	0.65	0.65
	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 399 and name CB)	17.96	0.68	0.67
	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 400 and name CA)	17.50	0.73	0.74
	assign (segid 3A4 and resid 139 and name CA)	(segid 3A4 and resid 400 and name CB)	16.60	0.72	0.72
	assign (segid 3A4 and resid 139 and name N)	(segid 3A4 and resid 139 and name C)	2.48	0.05	0.04
50	assign (segid 3A4 and resid 139 and name N)	(segid 3A4 and resid 139 and name CA)	1.45	0.00	0.01
	assign (segid 3A4 and resid 139 and name N)	(segid 3A4 and resid 139 and name O)	3.57	0.06	0.05
	assign (segid 3A4 and resid 139 and name N)	(segid 3A4 and resid 140 and name C)	5.03	0.16	0.17
	assign (segid 3A4 and resid 139 and name N)	(segid 3A4 and resid 140 and name CA)	4.21	0.08	0.08
	assign (segid 3A4 and resid 139 and name N)	(segid 3A4 and resid 140 and name CB)	4.81	0.07	0.06
55	assign (segid 3A4 and resid 139 and name N)	(segid 3A4 and resid 140 and name N)	2.78	0.09	0.09
	assign (segid 3A4 and resid 139 and name N)	(segid 3A4 and resid 140 and name O)	4.95	0.27	0.27
	assign (segid 3A4 and resid 139 and name N)	(segid 3A4 and resid 141 and name CA)	7.25	0.18	0.19
	assign (segid 3A4 and resid 139 and name N)	(segid 3A4 and resid 141 and name N)	6.18	0.16	0.17
	assign (segid 3A4 and resid 139 and name N)	(segid 3A4 and resid 219 and name C)	5.93	0.40	0.39
60	assign (segid 3A4 and resid 139 and name N)	(segid 3A4 and resid 219 and name CA)	5.33	0.29	0.30
	assign (segid 3A4 and resid 139 and name N)	(segid 3A4 and resid 219 and name CB)	4.03	0.20	0.20
	assign (segid 3A4 and resid 139 and name N)	(segid 3A4 and resid 219 and name CG)	4.34	0.15	0.15
	assign (segid 3A4 and resid 139 and name N)	(segid 3A4 and resid 219 and name N)	6.33	0.15	0.15
	assign (segid 3A4 and resid 139 and name N)	(segid 3A4 and resid 219 and name O)	6.90	0.31	0.30
65	assign (segid 3A4 and resid 139 and name N)	(segid 3A4 and resid 220 and name CB)	6.75	0.66	0.65
	assign (segid 3A4 and resid 139 and name N)	(segid 3A4 and resid 220 and name N)	5.70	0.58	0.59
	assign (segid 3A4 and resid 139 and name N)	(segid 3A4 and resid 221 and name CB)	6.03	0.61	0.61
	assign (segid 3A4 and resid 139 and name N)	(segid 3A4 and resid 221 and name N)	6.10	0.64	0.64
	assign (segid 3A4 and resid 139 and name N)	(segid 3A4 and resid 221 and name C)	3.47	0.23	0.24
70	assign (segid 3A4 and resid 139 and name O)	(segid 3A4 and resid 140 and name CA)	2.78	0.04	0.03
	assign (segid 3A4 and resid 139 and name O)	(segid 3A4 and resid 140 and name CB)	4.09	0.14	0.14
	assign (segid 3A4 and resid 139 and name O)	(segid 3A4 and resid 140 and name N)	2.23	0.01	0.02
	assign (segid 3A4 and resid 139 and name O)	(segid 3A4 and resid 140 and name O)	4.10	0.26	0.26
	assign (segid 3A4 and resid 139 and name O)	(segid 3A4 and resid 141 and name C)	6.33	0.40	0.39
75	assign (segid 3A4 and resid 139 and name O)	(segid 3A4 and resid 141 and name CA)	5.14	0.44	0.45
	assign (segid 3A4 and resid 139 and name O)	(segid 3A4 and resid 141 and name CB)	5.60	0.44	0.44
	assign (segid 3A4 and resid 139 and name O)	(segid 3A4 and resid 141 and name N)	3.99	0.38	0.38
	assign (segid 3A4 and resid 139 and name O)	(segid 3A4 and resid 141 and name O)	6.65	0.39	0.39
	assign (segid 3A4 and resid 139 and name O)	(segid 3A4 and resid 219 and name CB)	6.12	0.54	0.55
80	assign (segid 3A4 and resid 139 and name O)	(segid 3A4 and resid 219 and name CG)	5.88	0.62	0.63
	assign (segid 3A4 and resid 13 and name C)	(segid 3A4 and resid 13 and name CB)	2.50	0.03	0.02
	assign (segid 3A4 and resid 13 and name C)	(segid 3A4 and resid 13 and name O)	1.23	0.00	0.00
	assign (segid 3A4 and resid 13 and name C)	(segid 3A4 and resid 19 and name N)	6.27	1.15	1.14

	assign (segid 3A4 and resid 13 and name CA) (segid 3A4 and resid 13 and name C)	1.52	0.01	0.01
	assign (segid 3A4 and resid 13 and name CA) (segid 3A4 and resid 13 and name CB)	1.53	0.01	0.01
	assign (segid 3A4 and resid 13 and name CA) (segid 3A4 and resid 13 and name O)	2.39	0.02	0.01
	assign (segid 3A4 and resid 13 and name CA) (segid 3A4 and resid 19 and name CA)	7.75	1.35	1.35
5	assign (segid 3A4 and resid 13 and name CA) (segid 3A4 and resid 19 and name CB)	8.88	1.57	1.58
	assign (segid 3A4 and resid 13 and name CA) (segid 3A4 and resid 20 and name CA)	9.33	0.75	0.74
	assign (segid 3A4 and resid 13 and name CA) (segid 3A4 and resid 20 and name CB)	10.72	0.73	0.73
	assign (segid 3A4 and resid 13 and name CA) (segid 3A4 and resid 21 and name CA)	8.89	1.08	1.09
	assign (segid 3A4 and resid 13 and name CA) (segid 3A4 and resid 21 and name CB)	7.67	1.23	1.22
10	assign (segid 3A4 and resid 13 and name CA) (segid 3A4 and resid 22 and name CA)	11.30	1.45	1.46
	assign (segid 3A4 and resid 13 and name CA) (segid 3A4 and resid 23 and name CA)	11.41	1.89	1.89
	assign (segid 3A4 and resid 13 and name CA) (segid 3A4 and resid 23 and name CB)	10.76	2.00	2.01
	assign (segid 3A4 and resid 13 and name CA) (segid 3A4 and resid 30 and name CA)	14.82	1.66	1.65
	assign (segid 3A4 and resid 13 and name CA) (segid 3A4 and resid 317 and name CA)	18.05	1.24	1.24
	assign (segid 3A4 and resid 13 and name CA) (segid 3A4 and resid 31 and name CA)	12.56	1.35	1.35
15	assign (segid 3A4 and resid 13 and name CA) (segid 3A4 and resid 31 and name CB)	13.27	1.18	1.18
	assign (segid 3A4 and resid 13 and name CA) (segid 3A4 and resid 32 and name CA)	10.05	1.35	1.36
	assign (segid 3A4 and resid 13 and name CA) (segid 3A4 and resid 32 and name CB)	9.01	1.56	1.56
	assign (segid 3A4 and resid 13 and name CA) (segid 3A4 and resid 331 and name CB)	16.61	1.32	1.32
20	assign (segid 3A4 and resid 13 and name CA) (segid 3A4 and resid 335 and name CA)	16.30	1.37	1.37
	assign (segid 3A4 and resid 13 and name CA) (segid 3A4 and resid 33 and name CA)	10.37	0.97	0.96
	assign (segid 3A4 and resid 13 and name CA) (segid 3A4 and resid 33 and name CB)	11.72	0.92	0.92
	assign (segid 3A4 and resid 13 and name CA) (segid 3A4 and resid 343 and name CA)	15.71	1.30	1.29
	assign (segid 3A4 and resid 13 and name CA) (segid 3A4 and resid 343 and name CB)	16.05	1.17	1.17
25	assign (segid 3A4 and resid 13 and name CA) (segid 3A4 and resid 344 and name CA)	14.01	1.45	1.44
	assign (segid 3A4 and resid 13 and name CA) (segid 3A4 and resid 344 and name CB)	13.36	1.68	1.67
	assign (segid 3A4 and resid 13 and name CA) (segid 3A4 and resid 345 and name CA)	13.58	0.97	0.97
	assign (segid 3A4 and resid 13 and name CA) (segid 3A4 and resid 345 and name CB)	14.81	0.78	0.77
	assign (segid 3A4 and resid 13 and name CA) (segid 3A4 and resid 346 and name CA)	11.81	1.07	1.06
30	assign (segid 3A4 and resid 13 and name CA) (segid 3A4 and resid 346 and name CB)	10.45	1.20	1.19
	assign (segid 3A4 and resid 13 and name CA) (segid 3A4 and resid 347 and name CA)	14.37	0.74	0.74
	assign (segid 3A4 and resid 13 and name CA) (segid 3A4 and resid 347 and name CB)	15.75	0.76	0.76
	assign (segid 3A4 and resid 13 and name CA) (segid 3A4 and resid 348 and name CA)	13.25	0.96	0.96
	assign (segid 3A4 and resid 13 and name CA) (segid 3A4 and resid 349 and name CA)	10.31	1.03	1.03
35	assign (segid 3A4 and resid 13 and name CA) (segid 3A4 and resid 349 and name CB)	9.22	1.11	1.11
	assign (segid 3A4 and resid 13 and name CA) (segid 3A4 and resid 34 and name CA)	8.38	1.38	1.39
	assign (segid 3A4 and resid 13 and name CA) (segid 3A4 and resid 34 and name CB)	7.05	1.42	1.41
	assign (segid 3A4 and resid 13 and name CA) (segid 3A4 and resid 350 and name CA)	12.68	1.28	1.29
40	assign (segid 3A4 and resid 13 and name CA) (segid 3A4 and resid 350 and name CB)	13.67	1.19	1.18
	assign (segid 3A4 and resid 13 and name CA) (segid 3A4 and resid 351 and name CA)	14.94	1.26	1.26
	assign (segid 3A4 and resid 13 and name CA) (segid 3A4 and resid 352 and name CA)	12.85	1.59	1.59
	assign (segid 3A4 and resid 13 and name CA) (segid 3A4 and resid 352 and name CB)	12.14	1.52	1.51
	assign (segid 3A4 and resid 13 and name CA) (segid 3A4 and resid 353 and name CA)	12.07	2.07	2.07
	assign (segid 3A4 and resid 13 and name CA) (segid 3A4 and resid 353 and name CB)	12.40	2.17	2.17
45	assign (segid 3A4 and resid 13 and name CA) (segid 3A4 and resid 354 and name CA)	13.63	2.35	2.36
	assign (segid 3A4 and resid 13 and name CA) (segid 3A4 and resid 354 and name CB)	13.13	2.43	2.43
	assign (segid 3A4 and resid 13 and name CA) (segid 3A4 and resid 355 and name CA)	14.81	2.91	2.90
	assign (segid 3A4 and resid 13 and name CA) (segid 3A4 and resid 35 and name CA)	10.37	1.55	1.54
	assign (segid 3A4 and resid 13 and name CA) (segid 3A4 and resid 360 and name CA)	16.03	1.76	1.75
50	assign (segid 3A4 and resid 13 and name CA) (segid 3A4 and resid 360 and name CB)	14.71	1.77	1.77
	assign (segid 3A4 and resid 13 and name CA) (segid 3A4 and resid 361 and name CA)	16.27	1.48	1.49
	assign (segid 3A4 and resid 13 and name CA) (segid 3A4 and resid 361 and name CB)	15.63	1.47	1.48
	assign (segid 3A4 and resid 13 and name CA) (segid 3A4 and resid 36 and name CA)	13.77	1.64	1.63
	assign (segid 3A4 and resid 13 and name CA) (segid 3A4 and resid 37 and name CA)	15.39	1.46	1.46
	assign (segid 3A4 and resid 13 and name CA) (segid 3A4 and resid 37 and name CB)	15.29	1.47	1.46
55	assign (segid 3A4 and resid 13 and name CA) (segid 3A4 and resid 38 and name CA)	14.21	1.20	1.20
	assign (segid 3A4 and resid 13 and name CA) (segid 3A4 and resid 38 and name CB)	12.97	1.16	1.15
	assign (segid 3A4 and resid 13 and name CA) (segid 3A4 and resid 39 and name CA)	14.94	1.19	1.19
	assign (segid 3A4 and resid 13 and name CA) (segid 3A4 and resid 39 and name CB)	14.40	1.22	1.21
60	assign (segid 3A4 and resid 13 and name CA) (segid 3A4 and resid 42 and name CB)	17.16	0.84	0.83
	assign (segid 3A4 and resid 13 and name CB) (segid 3A4 and resid 19 and name CA)	8.08	1.30	1.30
	assign (segid 3A4 and resid 13 and name CB) (segid 3A4 and resid 19 and name CB)	9.28	1.41	1.41
	assign (segid 3A4 and resid 13 and name CB) (segid 3A4 and resid 20 and name CA)	9.22	1.13	1.13
	assign (segid 3A4 and resid 13 and name CB) (segid 3A4 and resid 20 and name CB)	10.62	1.05	1.05
65	assign (segid 3A4 and resid 13 and name CB) (segid 3A4 and resid 21 and name CA)	8.62	1.59	1.60
	assign (segid 3A4 and resid 13 and name CB) (segid 3A4 and resid 21 and name CB)	7.45	1.69	1.70
	assign (segid 3A4 and resid 13 and name CB) (segid 3A4 and resid 22 and name CA)	10.75	2.04	2.04
	assign (segid 3A4 and resid 13 and name CB) (segid 3A4 and resid 23 and name CA)	10.64	2.48	2.48
	assign (segid 3A4 and resid 13 and name CB) (segid 3A4 and resid 23 and name CB)	9.91	2.61	2.61
70	assign (segid 3A4 and resid 13 and name CB) (segid 3A4 and resid 31 and name CA)	11.85	2.03	2.04
	assign (segid 3A4 and resid 13 and name CB) (segid 3A4 and resid 31 and name CB)	12.63	1.85	1.86
	assign (segid 3A4 and resid 13 and name CB) (segid 3A4 and resid 32 and name CA)	9.29	2.04	2.03
	assign (segid 3A4 and resid 13 and name CB) (segid 3A4 and resid 32 and name CB)	8.18	2.22	2.22
	assign (segid 3A4 and resid 13 and name CB) (segid 3A4 and resid 331 and name CB)	16.40	1.23	1.24
75	assign (segid 3A4 and resid 13 and name CB) (segid 3A4 and resid 335 and name CA)	16.29	1.21	1.21
	assign (segid 3A4 and resid 13 and name CB) (segid 3A4 and resid 33 and name CA)	9.88	1.53	1.53
	assign (segid 3A4 and resid 13 and name CB) (segid 3A4 and resid 33 and name CB)	11.25	1.44	1.44
	assign (segid 3A4 and resid 13 and name CB) (segid 3A4 and resid 344 and name CA)	13.12	2.15	2.15
	assign (segid 3A4 and resid 13 and name CB) (segid 3A4 and resid 344 and name CB)	12.42	2.36	2.35
80	assign (segid 3A4 and resid 13 and name CB) (segid 3A4 and resid 345 and name CA)	12.86	1.64	1.64
	assign (segid 3A4 and resid 13 and name CB) (segid 3A4 and resid 345 and name CB)	14.13	1.45	1.45
	assign (segid 3A4 and resid 13 and name CB) (segid 3A4 and resid 346 and name CA)	11.12	1.66	1.65
	assign (segid 3A4 and resid 13 and name CB) (segid 3A4 and resid 346 and name CB)	9.75	1.77	1.77

assign (segid 3A4 and resid 13 and name CB) (segid 3A4 and resid 347 and name CA) 13.82 1.28 1.27
 assign (segid 3A4 and resid 13 and name CB) (segid 3A4 and resid 347 and name CB) 15.16 1.29 1.28
 assign (segid 3A4 and resid 13 and name CB) (segid 3A4 and resid 348 and name CA) 12.60 1.38 1.37
 assign (segid 3A4 and resid 13 and name CB) (segid 3A4 and resid 349 and name CA) 10.03 1.48 1.47
 assign (segid 3A4 and resid 13 and name CB) (segid 3A4 and resid 349 and name CB) 8.89 1.60 1.60
 5 assign (segid 3A4 and resid 13 and name CB) (segid 3A4 and resid 34 and name CA) 8.11 1.85 1.84
 assign (segid 3A4 and resid 13 and name CB) (segid 3A4 and resid 34 and name CB) 6.84 1.87 1.87
 assign (segid 3A4 and resid 13 and name CB) (segid 3A4 and resid 350 and name CA) 12.50 1.57 1.57
 assign (segid 3A4 and resid 13 and name CB) (segid 3A4 and resid 350 and name CB) 13.42 1.46 1.46
 10 assign (segid 3A4 and resid 13 and name CB) (segid 3A4 and resid 351 and name CA) 14.81 1.51 1.50
 assign (segid 3A4 and resid 13 and name CB) (segid 3A4 and resid 352 and name CA) 12.92 1.84 1.84
 assign (segid 3A4 and resid 13 and name CB) (segid 3A4 and resid 352 and name CB) 12.17 1.77 1.77
 assign (segid 3A4 and resid 13 and name CB) (segid 3A4 and resid 353 and name CA) 12.34 2.28 2.28
 assign (segid 3A4 and resid 13 and name CB) (segid 3A4 and resid 353 and name CB) 12.63 2.36 2.36
 15 assign (segid 3A4 and resid 13 and name CB) (segid 3A4 and resid 354 and name CA) 14.13 2.64 2.63
 assign (segid 3A4 and resid 13 and name CB) (segid 3A4 and resid 354 and name CB) 13.70 2.75 2.76
 assign (segid 3A4 and resid 13 and name CB) (segid 3A4 and resid 35 and name CA) 10.44 1.73 1.73
 assign (segid 3A4 and resid 13 and name CB) (segid 3A4 and resid 360 and name CB) 14.98 2.08 2.09
 assign (segid 3A4 and resid 13 and name CB) (segid 3A4 and resid 361 and name CB) 15.90 1.80 1.79
 20 assign (segid 3A4 and resid 13 and name CB) (segid 3A4 and resid 36 and name CA) 13.73 1.83 1.84
 assign (segid 3A4 and resid 13 and name CB) (segid 3A4 and resid 37 and name CA) 15.46 1.52 1.51
 assign (segid 3A4 and resid 13 and name CB) (segid 3A4 and resid 37 and name CB) 15.45 1.42 1.43
 assign (segid 3A4 and resid 13 and name CB) (segid 3A4 and resid 382 and name CB) 17.68 1.61 1.62
 assign (segid 3A4 and resid 13 and name CB) (segid 3A4 and resid 38 and name CA) 14.10 1.38 1.38
 25 assign (segid 3A4 and resid 13 and name CB) (segid 3A4 and resid 38 and name CB) 12.87 1.34 1.34
 assign (segid 3A4 and resid 13 and name CB) (segid 3A4 and resid 39 and name CA) 14.59 1.57 1.56
 assign (segid 3A4 and resid 13 and name CB) (segid 3A4 and resid 39 and name CB) 14.02 1.62 1.63
 assign (segid 3A4 and resid 13 and name CB) (segid 3A4 and resid 42 and name CB) 16.68 1.33 1.34
 assign (segid 3A4 and resid 13 and name N) (segid 3A4 and resid 13 and name C) 2.47 0.01 0.02
 30 assign (segid 3A4 and resid 13 and name N) (segid 3A4 and resid 13 and name CA) 1.46 0.01 0.00
 assign (segid 3A4 and resid 13 and name N) (segid 3A4 and resid 13 and name CB) 2.44 0.01 0.01
 assign (segid 3A4 and resid 13 and name N) (segid 3A4 and resid 13 and name O) 3.50 0.05 0.06
 assign (segid 3A4 and resid 13 and name O) (segid 3A4 and resid 13 and name CB) 3.27 0.07 0.08
 assign (segid 3A4 and resid 13 and name O) (segid 3A4 and resid 19 and name N) 5.65 1.22 1.23
 35 assign (segid 3A4 and resid 140 and name C) (segid 3A4 and resid 140 and name CB) 2.50 0.01 0.02
 assign (segid 3A4 and resid 140 and name C) (segid 3A4 and resid 140 and name O) 1.23 0.00 0.01
 assign (segid 3A4 and resid 140 and name C) (segid 3A4 and resid 141 and name C) 3.22 0.12 0.13
 assign (segid 3A4 and resid 140 and name C) (segid 3A4 and resid 141 and name CA) 2.45 0.01 0.02
 assign (segid 3A4 and resid 140 and name C) (segid 3A4 and resid 141 and name CB) 3.58 0.07 0.08
 40 assign (segid 3A4 and resid 140 and name C) (segid 3A4 and resid 141 and name N) 1.33 0.00 0.01
 assign (segid 3A4 and resid 140 and name C) (segid 3A4 and resid 141 and name O) 3.51 0.24 0.24
 assign (segid 3A4 and resid 140 and name CA) (segid 3A4 and resid 140 and name CB) 1.53 0.01 0.01
 assign (segid 3A4 and resid 140 and name CA) (segid 3A4 and resid 140 and name O) 2.39 0.01 0.02
 45 assign (segid 3A4 and resid 140 and name CA) (segid 3A4 and resid 141 and name C) 4.56 0.06 0.07
 assign (segid 3A4 and resid 140 and name CA) (segid 3A4 and resid 141 and name CA) 3.84 0.03 0.03
 assign (segid 3A4 and resid 140 and name CA) (segid 3A4 and resid 141 and name CB) 4.76 0.04 0.03
 assign (segid 3A4 and resid 140 and name CA) (segid 3A4 and resid 141 and name N) 2.45 0.03 0.04
 assign (segid 3A4 and resid 140 and name CA) (segid 3A4 and resid 141 and name O) 4.58 0.21 0.22
 50 assign (segid 3A4 and resid 140 and name CA) (segid 3A4 and resid 141 and name CA) 9.20 2.95 2.95
 assign (segid 3A4 and resid 140 and name CA) (segid 3A4 and resid 147 and name CB) 10.24 2.77 2.78
 assign (segid 3A4 and resid 140 and name CA) (segid 3A4 and resid 148 and name CA) 9.73 1.51 1.51
 assign (segid 3A4 and resid 140 and name CA) (segid 3A4 and resid 149 and name CA) 8.63 1.87 1.88
 assign (segid 3A4 and resid 140 and name CA) (segid 3A4 and resid 149 and name CB) 7.75 2.09 2.09
 55 assign (segid 3A4 and resid 140 and name CA) (segid 3A4 and resid 150 and name CA) 10.33 2.93 2.93
 assign (segid 3A4 and resid 140 and name CA) (segid 3A4 and resid 151 and name CA) 12.94 1.94 1.94
 assign (segid 3A4 and resid 140 and name CA) (segid 3A4 and resid 152 and name CA) 12.44 1.43 1.42
 assign (segid 3A4 and resid 140 and name CA) (segid 3A4 and resid 152 and name CB) 11.70 1.14 1.14
 assign (segid 3A4 and resid 140 and name CA) (segid 3A4 and resid 153 and name CA) 12.10 2.72 2.72
 60 assign (segid 3A4 and resid 140 and name CA) (segid 3A4 and resid 153 and name CB) 11.20 3.17 3.16
 assign (segid 3A4 and resid 140 and name CA) (segid 3A4 and resid 155 and name CB) 16.44 1.59 1.59
 assign (segid 3A4 and resid 140 and name CA) (segid 3A4 and resid 156 and name CB) 15.06 2.24 2.24
 assign (segid 3A4 and resid 140 and name CA) (segid 3A4 and resid 193 and name CA) 15.79 1.07 1.07
 assign (segid 3A4 and resid 140 and name CA) (segid 3A4 and resid 193 and name CB) 16.02 1.05 1.04
 65 assign (segid 3A4 and resid 140 and name CA) (segid 3A4 and resid 194 and name CA) 13.25 1.19 1.19
 assign (segid 3A4 and resid 140 and name CA) (segid 3A4 and resid 194 and name CB) 13.59 1.29 1.28
 assign (segid 3A4 and resid 140 and name CA) (segid 3A4 and resid 195 and name CA) 14.50 1.13 1.13
 assign (segid 3A4 and resid 140 and name CA) (segid 3A4 and resid 195 and name CB) 15.96 1.14 1.14
 assign (segid 3A4 and resid 140 and name CA) (segid 3A4 and resid 196 and name CA) 14.30 0.83 0.84
 70 assign (segid 3A4 and resid 140 and name CA) (segid 3A4 and resid 196 and name CB) 15.08 0.80 0.81
 assign (segid 3A4 and resid 140 and name CA) (segid 3A4 and resid 197 and name CA) 10.69 0.86 0.86
 assign (segid 3A4 and resid 140 and name CA) (segid 3A4 and resid 197 and name CB) 10.19 0.97 0.96
 assign (segid 3A4 and resid 140 and name CA) (segid 3A4 and resid 198 and name CA) 9.96 0.90 0.91
 assign (segid 3A4 and resid 140 and name CA) (segid 3A4 and resid 198 and name CB) 10.59 1.00 1.01
 75 assign (segid 3A4 and resid 140 and name CA) (segid 3A4 and resid 199 and name CA) 12.76 0.74 0.74
 assign (segid 3A4 and resid 140 and name CA) (segid 3A4 and resid 199 and name CB) 14.10 0.78 0.79
 assign (segid 3A4 and resid 140 and name CA) (segid 3A4 and resid 200 and name CA) 11.58 0.73 0.72
 assign (segid 3A4 and resid 140 and name CA) (segid 3A4 and resid 201 and name CA) 8.47 0.71 0.71
 assign (segid 3A4 and resid 140 and name CA) (segid 3A4 and resid 201 and name CB) 7.35 0.64 0.64
 80 assign (segid 3A4 and resid 140 and name CA) (segid 3A4 and resid 202 and name CA) 11.14 0.65 0.66
 assign (segid 3A4 and resid 140 and name CA) (segid 3A4 and resid 202 and name CB) 12.08 0.67 0.68
 assign (segid 3A4 and resid 140 and name CA) (segid 3A4 and resid 203 and name CA) 13.52 0.66 0.65
 assign (segid 3A4 and resid 140 and name CA) (segid 3A4 and resid 203 and name CB) 14.11 0.64 0.64

	assign (segid 3A4 and resid 140 and name CA)	(segid 3A4 and resid 204 and name CA)	11.65	0.62	0.62
	assign (segid 3A4 and resid 140 and name CA)	(segid 3A4 and resid 204 and name CB)	10.51	0.61	0.60
	assign (segid 3A4 and resid 140 and name CA)	(segid 3A4 and resid 205 and name CA)	11.03	0.63	0.62
	assign (segid 3A4 and resid 140 and name CA)	(segid 3A4 and resid 205 and name CB)	10.25	0.61	0.62
5	assign (segid 3A4 and resid 140 and name CA)	(segid 3A4 and resid 206 and name CA)	14.70	0.59	0.59
	assign (segid 3A4 and resid 140 and name CA)	(segid 3A4 and resid 206 and name CB)	15.46	0.59	0.58
	assign (segid 3A4 and resid 140 and name CA)	(segid 3A4 and resid 207 and name CA)	15.79	0.69	0.69
	assign (segid 3A4 and resid 140 and name CA)	(segid 3A4 and resid 207 and name CB)	15.75	0.71	0.72
	assign (segid 3A4 and resid 140 and name CA)	(segid 3A4 and resid 219 and name CA)	9.29	0.33	0.34
	assign (segid 3A4 and resid 140 and name CA)	(segid 3A4 and resid 219 and name CB)	7.86	0.32	0.33
10	assign (segid 3A4 and resid 140 and name CA)	(segid 3A4 and resid 220 and name CA)	10.61	0.68	0.69
	assign (segid 3A4 and resid 140 and name CA)	(segid 3A4 and resid 220 and name CB)	10.55	0.68	0.68
	assign (segid 3A4 and resid 140 and name CA)	(segid 3A4 and resid 221 and name CA)	9.83	0.95	0.95
	assign (segid 3A4 and resid 140 and name CA)	(segid 3A4 and resid 221 and name CB)	8.64	1.02	1.02
	assign (segid 3A4 and resid 140 and name CA)	(segid 3A4 and resid 222 and name CA)	11.63	0.63	0.64
15	assign (segid 3A4 and resid 140 and name CA)	(segid 3A4 and resid 222 and name CB)	11.46	0.54	0.55
	assign (segid 3A4 and resid 140 and name CA)	(segid 3A4 and resid 223 and name CA)	14.28	0.64	0.64
	assign (segid 3A4 and resid 140 and name CA)	(segid 3A4 and resid 223 and name CB)	14.33	0.66	0.65
	assign (segid 3A4 and resid 140 and name CA)	(segid 3A4 and resid 224 and name CA)	14.90	0.88	0.87
	assign (segid 3A4 and resid 140 and name CA)	(segid 3A4 and resid 224 and name CB)	14.19	0.88	0.88
20	assign (segid 3A4 and resid 140 and name CA)	(segid 3A4 and resid 225 and name CA)	15.12	0.93	0.93
	assign (segid 3A4 and resid 140 and name CA)	(segid 3A4 and resid 225 and name CB)	14.17	0.89	0.89
	assign (segid 3A4 and resid 140 and name CA)	(segid 3A4 and resid 226 and name CA)	17.62	0.78	0.78
	assign (segid 3A4 and resid 140 and name CA)	(segid 3A4 and resid 241 and name CA)	18.06	0.74	0.74
	assign (segid 3A4 and resid 140 and name CA)	(segid 3A4 and resid 244 and name CA)	15.56	0.90	0.89
25	assign (segid 3A4 and resid 140 and name CA)	(segid 3A4 and resid 244 and name CB)	15.21	0.79	0.79
	assign (segid 3A4 and resid 140 and name CA)	(segid 3A4 and resid 245 and name CA)	14.25	1.00	0.99
	assign (segid 3A4 and resid 140 and name CA)	(segid 3A4 and resid 245 and name CB)	14.89	1.03	1.02
	assign (segid 3A4 and resid 140 and name CA)	(segid 3A4 and resid 246 and name CA)	16.44	1.12	1.13
	assign (segid 3A4 and resid 140 and name CA)	(segid 3A4 and resid 247 and name CA)	15.35	1.01	1.01
30	assign (segid 3A4 and resid 140 and name CA)	(segid 3A4 and resid 247 and name CB)	15.53	0.93	0.93
	assign (segid 3A4 and resid 140 and name CA)	(segid 3A4 and resid 248 and name CA)	11.63	1.04	1.05
	assign (segid 3A4 and resid 140 and name CA)	(segid 3A4 and resid 248 and name CB)	10.80	1.03	1.03
	assign (segid 3A4 and resid 140 and name CA)	(segid 3A4 and resid 249 and name CA)	13.04	1.27	1.27
	assign (segid 3A4 and resid 140 and name CA)	(segid 3A4 and resid 250 and name CA)	15.37	1.23	1.23
35	assign (segid 3A4 and resid 140 and name CA)	(segid 3A4 and resid 250 and name CB)	16.44	1.20	1.21
	assign (segid 3A4 and resid 140 and name CA)	(segid 3A4 and resid 251 and name CA)	13.15	1.07	1.08
	assign (segid 3A4 and resid 140 and name CA)	(segid 3A4 and resid 251 and name CB)	12.37	0.96	0.96
	assign (segid 3A4 and resid 140 and name CA)	(segid 3A4 and resid 252 and name CA)	11.27	1.31	1.30
	assign (segid 3A4 and resid 140 and name CA)	(segid 3A4 and resid 252 and name CB)	10.58	1.36	1.36
40	assign (segid 3A4 and resid 140 and name CA)	(segid 3A4 and resid 253 and name CA)	14.65	1.40	1.41
	assign (segid 3A4 and resid 140 and name CA)	(segid 3A4 and resid 254 and name CA)	16.64	1.34	1.35
	assign (segid 3A4 and resid 140 and name CA)	(segid 3A4 and resid 255 and name CA)	14.78	1.66	1.66
	assign (segid 3A4 and resid 140 and name CA)	(segid 3A4 and resid 256 and name CA)	14.28	1.02	1.03
	assign (segid 3A4 and resid 140 and name CA)	(segid 3A4 and resid 257 and name CA)	17.68	1.07	1.07
45	assign (segid 3A4 and resid 140 and name CA)	(segid 3A4 and resid 259 and name CA)	18.61	0.45	0.45
	assign (segid 3A4 and resid 140 and name CA)	(segid 3A4 and resid 259 and name CB)	17.40	0.39	0.39
	assign (segid 3A4 and resid 140 and name CA)	(segid 3A4 and resid 260 and name CA)	18.74	0.50	0.50
	assign (segid 3A4 and resid 140 and name CA)	(segid 3A4 and resid 260 and name CB)	18.10	0.60	0.60
50	assign (segid 3A4 and resid 140 and name CA)	(segid 3A4 and resid 393 and name CA)	18.27	0.46	0.46
	assign (segid 3A4 and resid 140 and name CA)	(segid 3A4 and resid 396 and name CA)	17.49	0.40	0.40
	assign (segid 3A4 and resid 140 and name CA)	(segid 3A4 and resid 396 and name CB)	16.20	0.43	0.43
	assign (segid 3A4 and resid 140 and name CA)	(segid 3A4 and resid 397 and name CA)	18.86	0.34	0.35
	assign (segid 3A4 and resid 140 and name CA)	(segid 3A4 and resid 397 and name CB)	19.54	0.32	0.32
55	assign (segid 3A4 and resid 140 and name CA)	(segid 3A4 and resid 400 and name CA)	18.16	0.63	0.63
	assign (segid 3A4 and resid 140 and name CA)	(segid 3A4 and resid 400 and name CB)	17.13	0.57	0.57
	assign (segid 3A4 and resid 140 and name CB)	(segid 3A4 and resid 141 and name C)	4.94	0.12	0.12
	assign (segid 3A4 and resid 140 and name CB)	(segid 3A4 and resid 141 and name CA)	4.63	0.11	0.11
	assign (segid 3A4 and resid 140 and name CB)	(segid 3A4 and resid 141 and name CB)	5.65	0.13	0.14
60	assign (segid 3A4 and resid 140 and name CB)	(segid 3A4 and resid 141 and name N)	3.33	0.12	0.13
	assign (segid 3A4 and resid 140 and name CB)	(segid 3A4 and resid 141 and name O)	4.65	0.29	0.29
	assign (segid 3A4 and resid 140 and name CB)	(segid 3A4 and resid 147 and name CA)	9.04	2.52	2.51
	assign (segid 3A4 and resid 140 and name CB)	(segid 3A4 and resid 147 and name CB)	10.14	2.28	2.27
	assign (segid 3A4 and resid 140 and name CB)	(segid 3A4 and resid 148 and name CA)	9.39	1.10	1.10
	assign (segid 3A4 and resid 140 and name CB)	(segid 3A4 and resid 149 and name CA)	8.02	1.75	1.75
65	assign (segid 3A4 and resid 140 and name CB)	(segid 3A4 and resid 149 and name CB)	7.21	1.99	1.99
	assign (segid 3A4 and resid 140 and name CB)	(segid 3A4 and resid 150 and name CA)	9.46	3.00	3.01
	assign (segid 3A4 and resid 140 and name CB)	(segid 3A4 and resid 151 and name CA)	11.94	1.98	1.98
	assign (segid 3A4 and resid 140 and name CB)	(segid 3A4 and resid 152 and name CA)	11.39	1.49	1.50
	assign (segid 3A4 and resid 140 and name CB)	(segid 3A4 and resid 152 and name CB)	10.74	1.15	1.15
70	assign (segid 3A4 and resid 140 and name CB)	(segid 3A4 and resid 153 and name CA)	10.97	2.98	2.97
	assign (segid 3A4 and resid 140 and name CB)	(segid 3A4 and resid 153 and name CB)	10.08	3.45	3.45
	assign (segid 3A4 and resid 140 and name CB)	(segid 3A4 and resid 154 and name CA)	13.48	3.16	3.15
	assign (segid 3A4 and resid 140 and name CB)	(segid 3A4 and resid 155 and name CA)	15.34	2.17	2.17
	assign (segid 3A4 and resid 140 and name CB)	(segid 3A4 and resid 155 and name CB)	15.26	1.71	1.72
75	assign (segid 3A4 and resid 140 and name CB)	(segid 3A4 and resid 156 and name CA)	14.96	2.44	2.44
	assign (segid 3A4 and resid 140 and name CB)	(segid 3A4 and resid 156 and name CB)	13.92	2.46	2.47
	assign (segid 3A4 and resid 140 and name CB)	(segid 3A4 and resid 193 and name CA)	14.73	1.11	1.12
	assign (segid 3A4 and resid 140 and name CB)	(segid 3A4 and resid 193 and name CB)	14.93	1.12	1.12
80	assign (segid 3A4 and resid 140 and name CB)	(segid 3A4 and resid 194 and name CA)	12.15	1.30	1.29
	assign (segid 3A4 and resid 140 and name CB)	(segid 3A4 and resid 194 and name CB)	12.44	1.41	1.45
	assign (segid 3A4 and resid 140 and name CB)	(segid 3A4 and resid 195 and name CA)	13.56	1.16	1.15
	assign (segid 3A4 and resid 140 and name CB)	(segid 3A4 and resid 195 and name CB)	15.01	1.16	1.17

	assign (segid 3A4 and resid 140 and name CB)	(segid 3A4 and resid 196 and name CA)	13.49	0.75	0.75
	assign (segid 3A4 and resid 140 and name CB)	(segid 3A4 and resid 196 and name CB)	14.25	0.73	0.72
	assign (segid 3A4 and resid 140 and name CB)	(segid 3A4 and resid 197 and name CA)	9.89	0.79	0.78
	assign (segid 3A4 and resid 140 and name CB)	(segid 3A4 and resid 197 and name CB)	9.28	0.95	0.95
5	assign (segid 3A4 and resid 140 and name CB)	(segid 3A4 and resid 198 and name CA)	9.26	0.84	0.84
	assign (segid 3A4 and resid 140 and name CB)	(segid 3A4 and resid 198 and name CB)	9.82	1.02	1.02
	assign (segid 3A4 and resid 140 and name CB)	(segid 3A4 and resid 199 and name CA)	12.25	0.54	0.54
	assign (segid 3A4 and resid 140 and name CB)	(segid 3A4 and resid 199 and name CB)	13.54	0.59	0.60
	assign (segid 3A4 and resid 140 and name CB)	(segid 3A4 and resid 200 and name CA)	11.27	0.46	0.47
10	assign (segid 3A4 and resid 140 and name CB)	(segid 3A4 and resid 201 and name CA)	8.35	0.51	0.52
	assign (segid 3A4 and resid 140 and name CB)	(segid 3A4 and resid 201 and name CB)	7.14	0.47	0.46
	assign (segid 3A4 and resid 140 and name CB)	(segid 3A4 and resid 202 and name CA)	11.07	0.49	0.48
	assign (segid 3A4 and resid 140 and name CB)	(segid 3A4 and resid 202 and name CB)	11.89	0.55	0.55
	assign (segid 3A4 and resid 140 and name CB)	(segid 3A4 and resid 203 and name CA)	13.54	0.44	0.45
15	assign (segid 3A4 and resid 140 and name CB)	(segid 3A4 and resid 203 and name CB)	14.07	0.41	0.41
	assign (segid 3A4 and resid 140 and name CB)	(segid 3A4 and resid 204 and name CA)	11.94	0.55	0.55
	assign (segid 3A4 and resid 140 and name CB)	(segid 3A4 and resid 204 and name CB)	10.80	0.49	0.49
	assign (segid 3A4 and resid 140 and name CB)	(segid 3A4 and resid 205 and name CA)	11.46	0.62	0.62
	assign (segid 3A4 and resid 140 and name CB)	(segid 3A4 and resid 205 and name CB)	10.64	0.53	0.52
20	assign (segid 3A4 and resid 140 and name CB)	(segid 3A4 and resid 206 and name CA)	15.05	0.54	0.53
	assign (segid 3A4 and resid 140 and name CB)	(segid 3A4 and resid 206 and name CB)	15.70	0.44	0.45
	assign (segid 3A4 and resid 140 and name CB)	(segid 3A4 and resid 207 and name CA)	16.27	0.75	0.75
	assign (segid 3A4 and resid 140 and name CB)	(segid 3A4 and resid 207 and name CB)	16.20	0.84	0.84
	assign (segid 3A4 and resid 140 and name CB)	(segid 3A4 and resid 219 and name CA)	10.01	0.35	0.34
25	assign (segid 3A4 and resid 140 and name CB)	(segid 3A4 and resid 219 and name CB)	8.62	0.29	0.30
	assign (segid 3A4 and resid 140 and name CB)	(segid 3A4 and resid 220 and name CA)	10.89	0.78	0.77
	assign (segid 3A4 and resid 140 and name CB)	(segid 3A4 and resid 220 and name CB)	10.67	0.81	0.81
	assign (segid 3A4 and resid 140 and name CB)	(segid 3A4 and resid 221 and name CA)	9.99	0.92	0.93
	assign (segid 3A4 and resid 140 and name CB)	(segid 3A4 and resid 221 and name CB)	8.77	0.95	0.96
30	assign (segid 3A4 and resid 140 and name CB)	(segid 3A4 and resid 222 and name CA)	12.14	0.49	0.50
	assign (segid 3A4 and resid 140 and name CB)	(segid 3A4 and resid 222 and name CB)	12.12	0.38	0.38
	assign (segid 3A4 and resid 140 and name CB)	(segid 3A4 and resid 223 and name CA)	14.70	0.61	0.62
	assign (segid 3A4 and resid 140 and name CB)	(segid 3A4 and resid 223 and name CB)	14.73	0.66	0.66
	assign (segid 3A4 and resid 140 and name CB)	(segid 3A4 and resid 224 and name CA)	15.00	0.91	0.92
35	assign (segid 3A4 and resid 140 and name CB)	(segid 3A4 and resid 224 and name CB)	14.18	0.96	0.95
	assign (segid 3A4 and resid 140 and name CB)	(segid 3A4 and resid 225 and name CA)	15.31	0.88	0.87
	assign (segid 3A4 and resid 140 and name CB)	(segid 3A4 and resid 225 and name CB)	14.41	0.82	0.81
	assign (segid 3A4 and resid 140 and name CB)	(segid 3A4 and resid 226 and name CA)	18.00	0.70	0.69
	assign (segid 3A4 and resid 140 and name CB)	(segid 3A4 and resid 241 and name CA)	17.73	0.76	0.76
40	assign (segid 3A4 and resid 140 and name CB)	(segid 3A4 and resid 241 and name CB)	17.94	0.83	0.83
	assign (segid 3A4 and resid 140 and name CB)	(segid 3A4 and resid 244 and name CA)	15.19	0.96	0.96
	assign (segid 3A4 and resid 140 and name CB)	(segid 3A4 and resid 244 and name CB)	14.94	0.82	0.82
	assign (segid 3A4 and resid 140 and name CB)	(segid 3A4 and resid 245 and name CA)	13.64	1.08	1.08
	assign (segid 3A4 and resid 140 and name CB)	(segid 3A4 and resid 245 and name CB)	14.25	1.09	1.09
45	assign (segid 3A4 and resid 140 and name CB)	(segid 3A4 and resid 246 and name CA)	15.70	1.31	1.31
	assign (segid 3A4 and resid 140 and name CB)	(segid 3A4 and resid 247 and name CA)	14.76	1.25	1.26
	assign (segid 3A4 and resid 140 and name CB)	(segid 3A4 and resid 247 and name CB)	15.05	1.17	1.17
	assign (segid 3A4 and resid 140 and name CB)	(segid 3A4 and resid 248 and name CA)	11.01	1.28	1.29
	assign (segid 3A4 and resid 140 and name CB)	(segid 3A4 and resid 248 and name CB)	10.21	1.23	1.24
50	assign (segid 3A4 and resid 140 and name CB)	(segid 3A4 and resid 249 and name CA)	12.12	1.55	1.56
	assign (segid 3A4 and resid 140 and name CB)	(segid 3A4 and resid 250 and name CA)	14.53	1.61	1.62
	assign (segid 3A4 and resid 140 and name CB)	(segid 3A4 and resid 250 and name CB)	15.65	1.57	1.58
	assign (segid 3A4 and resid 140 and name CB)	(segid 3A4 and resid 251 and name CA)	12.48	1.50	1.50
	assign (segid 3A4 and resid 140 and name CB)	(segid 3A4 and resid 251 and name CB)	11.80	1.35	1.36
55	assign (segid 3A4 and resid 140 and name CB)	(segid 3A4 and resid 252 and name CA)	10.36	1.74	1.74
	assign (segid 3A4 and resid 140 and name CB)	(segid 3A4 and resid 252 and name CB)	9.59	1.76	1.76
	assign (segid 3A4 and resid 140 and name CB)	(segid 3A4 and resid 253 and name CA)	13.64	1.85	1.85
	assign (segid 3A4 and resid 140 and name CB)	(segid 3A4 and resid 254 and name CA)	15.80	1.82	1.83
	assign (segid 3A4 and resid 140 and name CB)	(segid 3A4 and resid 255 and name CA)	14.08	2.00	1.99
60	assign (segid 3A4 and resid 140 and name CB)	(segid 3A4 and resid 256 and name CA)	13.46	1.45	1.44
	assign (segid 3A4 and resid 140 and name CB)	(segid 3A4 and resid 257 and name CA)	16.78	1.53	1.53
	assign (segid 3A4 and resid 140 and name CB)	(segid 3A4 and resid 259 and name CB)	16.85	0.91	0.91
	assign (segid 3A4 and resid 140 and name CB)	(segid 3A4 and resid 260 and name CA)	18.07	0.94	0.94
	assign (segid 3A4 and resid 140 and name CB)	(segid 3A4 and resid 260 and name CB)	17.37	0.98	0.97
65	assign (segid 3A4 and resid 140 and name CB)	(segid 3A4 and resid 393 and name CA)	17.96	0.85	0.85
	assign (segid 3A4 and resid 140 and name CB)	(segid 3A4 and resid 396 and name CA)	17.43	0.56	0.56
	assign (segid 3A4 and resid 140 and name CB)	(segid 3A4 and resid 396 and name CB)	16.11	0.59	0.59
	assign (segid 3A4 and resid 140 and name CB)	(segid 3A4 and resid 397 and name CA)	18.60	0.62	0.61
	assign (segid 3A4 and resid 140 and name CB)	(segid 3A4 and resid 400 and name CA)	18.11	0.48	0.48
70	assign (segid 3A4 and resid 140 and name CB)	(segid 3A4 and resid 400 and name CB)	17.00	0.59	0.58
	assign (segid 3A4 and resid 140 and name N)	(segid 3A4 and resid 140 and name C)	2.44	0.04	0.03
	assign (segid 3A4 and resid 140 and name N)	(segid 3A4 and resid 140 and name CA)	1.46	0.02	0.01
	assign (segid 3A4 and resid 140 and name N)	(segid 3A4 and resid 140 and name CB)	2.45	0.03	0.04
	assign (segid 3A4 and resid 140 and name N)	(segid 3A4 and resid 140 and name O)	2.79	0.08	0.08
75	assign (segid 3A4 and resid 140 and name N)	(segid 3A4 and resid 141 and name C)	5.63	0.10	0.11
	assign (segid 3A4 and resid 140 and name N)	(segid 3A4 and resid 141 and name CA)	4.79	0.08	0.07
	assign (segid 3A4 and resid 140 and name N)	(segid 3A4 and resid 141 and name CB)	5.71	0.11	0.11
	assign (segid 3A4 and resid 140 and name N)	(segid 3A4 and resid 141 and name O)	3.55	0.08	0.07
	assign (segid 3A4 and resid 140 and name N)	(segid 3A4 and resid 141 and name N)	5.83	0.22	0.21
80	assign (segid 3A4 and resid 140 and name N)	(segid 3A4 and resid 219 and name CB)	6.48	0.29	0.29
	assign (segid 3A4 and resid 140 and name N)	(segid 3A4 and resid 219 and name CG)	6.51	0.24	0.24
	assign (segid 3A4 and resid 140 and name O)	(segid 3A4 and resid 140 and name CB)	3.12	0.12	0.12
	assign (segid 3A4 and resid 140 and name O)	(segid 3A4 and resid 141 and name C)	3.35	0.29	0.28

	assign (segid 3A4 and resid 140 and name O)	(segid 3A4 and resid 141 and name CA)	2.79	0.02	0.02
	assign (segid 3A4 and resid 140 and name O)	(segid 3A4 and resid 141 and name CB)	4.09	0.17	0.17
	assign (segid 3A4 and resid 140 and name O)	(segid 3A4 and resid 141 and name N)	2.25	0.02	0.01
	assign (segid 3A4 and resid 140 and name O)	(segid 3A4 and resid 141 and name O)	3.81	0.41	0.41
5	assign (segid 3A4 and resid 141 and name C)	(segid 3A4 and resid 141 and name CB)	2.49	0.03	0.03
	assign (segid 3A4 and resid 141 and name C)	(segid 3A4 and resid 141 and name O)	1.23	0.00	0.00
	assign (segid 3A4 and resid 141 and name CA)	(segid 3A4 and resid 141 and name C)	1.51	0.01	0.01
	assign (segid 3A4 and resid 141 and name CA)	(segid 3A4 and resid 141 and name CB)	1.51	0.02	0.02
	assign (segid 3A4 and resid 141 and name CA)	(segid 3A4 and resid 141 and name O)	2.39	0.01	0.01
10	assign (segid 3A4 and resid 141 and name CA)	(segid 3A4 and resid 147 and name CA)	6.80	3.45	3.44
	assign (segid 3A4 and resid 141 and name CA)	(segid 3A4 and resid 147 and name CB)	7.77	3.38	3.39
	assign (segid 3A4 and resid 141 and name CA)	(segid 3A4 and resid 148 and name CA)	7.52	2.33	2.34
	assign (segid 3A4 and resid 141 and name CA)	(segid 3A4 and resid 149 and name CA)	7.32	1.87	1.88
	assign (segid 3A4 and resid 141 and name CA)	(segid 3A4 and resid 149 and name CB)	6.63	1.78	1.77
	assign (segid 3A4 and resid 141 and name CA)	(segid 3A4 and resid 150 and name CA)	9.35	2.49	2.49
15	assign (segid 3A4 and resid 141 and name CA)	(segid 3A4 and resid 151 and name CA)	12.12	1.86	1.86
	assign (segid 3A4 and resid 141 and name CA)	(segid 3A4 and resid 152 and name CA)	12.12	1.37	1.38
	assign (segid 3A4 and resid 141 and name CA)	(segid 3A4 and resid 152 and name CB)	11.34	1.18	1.18
	assign (segid 3A4 and resid 141 and name CA)	(segid 3A4 and resid 153 and name CA)	12.31	2.03	2.03
	assign (segid 3A4 and resid 141 and name CA)	(segid 3A4 and resid 153 and name CB)	11.45	2.28	2.28
20	assign (segid 3A4 and resid 141 and name CA)	(segid 3A4 and resid 193 and name CA)	16.93	0.46	0.47
	assign (segid 3A4 and resid 141 and name CA)	(segid 3A4 and resid 193 and name CB)	16.91	0.49	0.48
	assign (segid 3A4 and resid 141 and name CA)	(segid 3A4 and resid 194 and name CA)	14.86	0.43	0.43
	assign (segid 3A4 and resid 141 and name CA)	(segid 3A4 and resid 194 and name CB)	15.30	0.45	0.45
25	assign (segid 3A4 and resid 141 and name CA)	(segid 3A4 and resid 195 and name CA)	16.62	0.49	0.50
	assign (segid 3A4 and resid 141 and name CA)	(segid 3A4 and resid 195 and name CB)	18.13	0.51	0.51
	assign (segid 3A4 and resid 141 and name CA)	(segid 3A4 and resid 196 and name CA)	16.00	0.43	0.43
	assign (segid 3A4 and resid 141 and name CA)	(segid 3A4 and resid 196 and name CB)	16.52	0.41	0.42
	assign (segid 3A4 and resid 141 and name CA)	(segid 3A4 and resid 197 and name CA)	12.25	0.43	0.43
30	assign (segid 3A4 and resid 141 and name CA)	(segid 3A4 and resid 197 and name CB)	11.60	0.42	0.41
	assign (segid 3A4 and resid 141 and name CA)	(segid 3A4 and resid 198 and name CA)	12.41	0.44	0.44
	assign (segid 3A4 and resid 141 and name CA)	(segid 3A4 and resid 198 and name CB)	13.19	0.43	0.44
	assign (segid 3A4 and resid 141 and name CA)	(segid 3A4 and resid 199 and name CA)	15.16	0.60	0.60
	assign (segid 3A4 and resid 141 and name CA)	(segid 3A4 and resid 199 and name CB)	16.39	0.63	0.62
35	assign (segid 3A4 and resid 141 and name CA)	(segid 3A4 and resid 200 and name CA)	13.46	0.90	0.90
	assign (segid 3A4 and resid 141 and name CA)	(segid 3A4 and resid 201 and name CA)	10.87	0.86	0.85
	assign (segid 3A4 and resid 141 and name CA)	(segid 3A4 and resid 201 and name CB)	9.96	0.63	0.63
	assign (segid 3A4 and resid 141 and name CA)	(segid 3A4 and resid 202 and name CA)	13.96	0.80	0.81
	assign (segid 3A4 and resid 141 and name CA)	(segid 3A4 and resid 202 and name CB)	14.98	0.69	0.69
40	assign (segid 3A4 and resid 141 and name CA)	(segid 3A4 and resid 203 and name CA)	15.85	1.11	1.12
	assign (segid 3A4 and resid 141 and name CA)	(segid 3A4 and resid 203 and name CB)	16.26	1.09	1.10
	assign (segid 3A4 and resid 141 and name CA)	(segid 3A4 and resid 204 and name CA)	13.57	1.35	1.36
	assign (segid 3A4 and resid 141 and name CA)	(segid 3A4 and resid 204 and name CB)	12.25	1.40	1.39
	assign (segid 3A4 and resid 141 and name CA)	(segid 3A4 and resid 205 and name CA)	13.49	1.21	1.21
45	assign (segid 3A4 and resid 141 and name CA)	(segid 3A4 and resid 205 and name CB)	12.95	1.09	1.10
	assign (segid 3A4 and resid 141 and name CA)	(segid 3A4 and resid 206 and name CA)	17.23	1.19	1.20
	assign (segid 3A4 and resid 141 and name CA)	(segid 3A4 and resid 206 and name CB)	18.04	1.17	1.16
	assign (segid 3A4 and resid 141 and name CA)	(segid 3A4 and resid 207 and name CA)	17.77	1.48	1.48
	assign (segid 3A4 and resid 141 and name CA)	(segid 3A4 and resid 207 and name CB)	17.56	1.49	1.49
50	assign (segid 3A4 and resid 141 and name CA)	(segid 3A4 and resid 219 and name CA)	11.81	0.53	0.54
	assign (segid 3A4 and resid 141 and name CA)	(segid 3A4 and resid 219 and name CB)	10.42	0.56	0.56
	assign (segid 3A4 and resid 141 and name CA)	(segid 3A4 and resid 220 and name CA)	13.61	0.42	0.42
	assign (segid 3A4 and resid 141 and name CA)	(segid 3A4 and resid 220 and name CB)	13.55	0.32	0.32
	assign (segid 3A4 and resid 141 and name CA)	(segid 3A4 and resid 221 and name CA)	13.09	0.81	0.80
55	assign (segid 3A4 and resid 141 and name CA)	(segid 3A4 and resid 221 and name CB)	11.92	0.90	0.91
	assign (segid 3A4 and resid 141 and name CA)	(segid 3A4 and resid 222 and name CA)	14.54	0.95	0.95
	assign (segid 3A4 and resid 141 and name CA)	(segid 3A4 and resid 222 and name CB)	14.17	1.00	1.01
	assign (segid 3A4 and resid 141 and name CA)	(segid 3A4 and resid 223 and name CA)	17.25	0.73	0.74
	assign (segid 3A4 and resid 141 and name CA)	(segid 3A4 and resid 223 and name CB)	17.26	0.67	0.67
60	assign (segid 3A4 and resid 141 and name CA)	(segid 3A4 and resid 224 and name CA)	18.13	0.71	0.72
	assign (segid 3A4 and resid 141 and name CA)	(segid 3A4 and resid 224 and name CB)	17.49	0.64	0.64
	assign (segid 3A4 and resid 141 and name CA)	(segid 3A4 and resid 225 and name CA)	17.21	1.10	1.09
	assign (segid 3A4 and resid 141 and name CA)	(segid 3A4 and resid 224 and name CB)	18.75	0.43	0.42
	assign (segid 3A4 and resid 141 and name CA)	(segid 3A4 and resid 244 and name CB)	18.39	0.45	0.46
65	assign (segid 3A4 and resid 141 and name CA)	(segid 3A4 and resid 245 and name CA)	17.22	0.40	0.40
	assign (segid 3A4 and resid 141 and name CA)	(segid 3A4 and resid 245 and name CB)	17.74	0.47	0.48
	assign (segid 3A4 and resid 141 and name CA)	(segid 3A4 and resid 247 and name CA)	18.42	0.36	0.35
	assign (segid 3A4 and resid 141 and name CA)	(segid 3A4 and resid 247 and name CB)	18.68	0.37	0.36
	assign (segid 3A4 and resid 141 and name CA)	(segid 3A4 and resid 248 and name CA)	14.65	0.35	0.35
70	assign (segid 3A4 and resid 141 and name CA)	(segid 3A4 and resid 248 and name CB)	13.86	0.36	0.37
	assign (segid 3A4 and resid 141 and name CA)	(segid 3A4 and resid 249 and name CA)	15.63	0.37	0.38
	assign (segid 3A4 and resid 141 and name CA)	(segid 3A4 and resid 250 and name CA)	17.96	0.38	0.39
	assign (segid 3A4 and resid 141 and name CA)	(segid 3A4 and resid 250 and name CB)	19.14	0.32	0.32
	assign (segid 3A4 and resid 141 and name CA)	(segid 3A4 and resid 251 and name CA)	15.72	0.39	0.40
75	assign (segid 3A4 and resid 141 and name CA)	(segid 3A4 and resid 251 and name CB)	15.08	0.37	0.37
	assign (segid 3A4 and resid 141 and name CA)	(segid 3A4 and resid 252 and name CA)	13.39	0.58	0.58
	assign (segid 3A4 and resid 141 and name CA)	(segid 3A4 and resid 252 and name CB)	12.71	0.53	0.53
	assign (segid 3A4 and resid 141 and name CA)	(segid 3A4 and resid 253 and name CA)	16.48	0.68	0.69
	assign (segid 3A4 and resid 141 and name CA)	(segid 3A4 and resid 256 and name CA)	15.31	1.31	1.31
80	assign (segid 3A4 and resid 141 and name CA)	(segid 3A4 and resid 259 and name CB)	18.19	1.15	1.15
	assign (segid 3A4 and resid 141 and name CA)	(segid 3A4 and resid 396 and name CB)	17.89	1.11	1.10
	assign (segid 3A4 and resid 141 and name CA)	(segid 3A4 and resid 400 and name CB)	17.68	1.49	1.49
	assign (segid 3A4 and resid 141 and name CB)	(segid 3A4 and resid 147 and name CA)	7.59	3.49	3.49

	assign (segid 3A4 and resid 141 and name CB)	(segid 3A4 and resid 147 and name CB)	8.48	3.48	3.48
	assign (segid 3A4 and resid 141 and name CB)	(segid 3A4 and resid 148 and name CA)	7.78	2.87	2.87
	assign (segid 3A4 and resid 141 and name CB)	(segid 3A4 and resid 149 and name CA)	7.72	2.28	2.28
	assign (segid 3A4 and resid 141 and name CB)	(segid 3A4 and resid 149 and name CB)	6.95	2.17	2.17
	assign (segid 3A4 and resid 141 and name CB)	(segid 3A4 and resid 150 and name CA)	10.12	2.56	2.57
5	assign (segid 3A4 and resid 141 and name CB)	(segid 3A4 and resid 151 and name CA)	12.79	2.12	2.12
	assign (segid 3A4 and resid 141 and name CB)	(segid 3A4 and resid 152 and name CA)	12.66	1.76	1.76
	assign (segid 3A4 and resid 141 and name CB)	(segid 3A4 and resid 152 and name CB)	11.78	1.60	1.59
	assign (segid 3A4 and resid 141 and name CB)	(segid 3A4 and resid 153 and name CA)	13.00	2.28	2.28
	assign (segid 3A4 and resid 141 and name CB)	(segid 3A4 and resid 153 and name CB)	12.17	2.48	2.47
10	assign (segid 3A4 and resid 141 and name CB)	(segid 3A4 and resid 193 and name CA)	17.28	0.81	0.81
	assign (segid 3A4 and resid 141 and name CB)	(segid 3A4 and resid 193 and name CB)	17.26	0.70	0.69
	assign (segid 3A4 and resid 141 and name CB)	(segid 3A4 and resid 194 and name CA)	15.39	0.83	0.84
	assign (segid 3A4 and resid 141 and name CB)	(segid 3A4 and resid 194 and name CB)	15.92	0.83	0.83
	assign (segid 3A4 and resid 141 and name CB)	(segid 3A4 and resid 195 and name CA)	17.09	0.97	0.98
15	assign (segid 3A4 and resid 141 and name CB)	(segid 3A4 and resid 196 and name CA)	16.24	1.03	1.02
	assign (segid 3A4 and resid 141 and name CB)	(segid 3A4 and resid 196 and name CB)	16.70	1.01	1.01
	assign (segid 3A4 and resid 141 and name CB)	(segid 3A4 and resid 197 and name CA)	12.52	1.02	1.01
	assign (segid 3A4 and resid 141 and name CB)	(segid 3A4 and resid 197 and name CB)	11.94	0.91	0.91
	assign (segid 3A4 and resid 141 and name CB)	(segid 3A4 and resid 198 and name CA)	12.86	0.92	0.92
20	assign (segid 3A4 and resid 141 and name CB)	(segid 3A4 and resid 198 and name CB)	13.74	0.85	0.84
	assign (segid 3A4 and resid 141 and name CB)	(segid 3A4 and resid 199 and name CA)	15.42	1.14	1.14
	assign (segid 3A4 and resid 141 and name CB)	(segid 3A4 and resid 199 and name CB)	16.62	1.20	1.19
	assign (segid 3A4 and resid 141 and name CB)	(segid 3A4 and resid 200 and name CA)	13.49	1.49	1.49
	assign (segid 3A4 and resid 141 and name CB)	(segid 3A4 and resid 201 and name CA)	11.07	1.32	1.31
25	assign (segid 3A4 and resid 141 and name CB)	(segid 3A4 and resid 201 and name CB)	10.30	1.07	1.07
	assign (segid 3A4 and resid 141 and name CB)	(segid 3A4 and resid 202 and name CA)	14.26	1.20	1.19
	assign (segid 3A4 and resid 141 and name CB)	(segid 3A4 and resid 202 and name CB)	15.32	1.10	1.09
	assign (segid 3A4 and resid 141 and name CB)	(segid 3A4 and resid 203 and name CA)	15.89	1.62	1.62
	assign (segid 3A4 and resid 141 and name CB)	(segid 3A4 and resid 203 and name CB)	16.25	1.66	1.66
30	assign (segid 3A4 and resid 141 and name CB)	(segid 3A4 and resid 204 and name CA)	13.47	1.87	1.87
	assign (segid 3A4 and resid 141 and name CB)	(segid 3A4 and resid 204 and name CB)	12.11	1.94	1.94
	assign (segid 3A4 and resid 141 and name CB)	(segid 3A4 and resid 205 and name CA)	13.62	1.56	1.55
	assign (segid 3A4 and resid 141 and name CB)	(segid 3A4 and resid 205 and name CB)	13.20	1.40	1.41
35	assign (segid 3A4 and resid 141 and name CB)	(segid 3A4 and resid 206 and name CA)	17.32	1.58	1.59
	assign (segid 3A4 and resid 141 and name CB)	(segid 3A4 and resid 219 and name CA)	12.48	0.52	0.52
	assign (segid 3A4 and resid 141 and name CB)	(segid 3A4 and resid 219 and name CB)	11.09	0.55	0.54
	assign (segid 3A4 and resid 141 and name CB)	(segid 3A4 and resid 220 and name CA)	14.40	0.40	0.39
	assign (segid 3A4 and resid 141 and name CB)	(segid 3A4 and resid 220 and name CB)	14.43	0.33	0.32
40	assign (segid 3A4 and resid 141 and name CB)	(segid 3A4 and resid 221 and name CA)	13.73	0.93	0.94
	assign (segid 3A4 and resid 141 and name CB)	(segid 3A4 and resid 221 and name CB)	12.55	1.08	1.08
	assign (segid 3A4 and resid 141 and name CB)	(segid 3A4 and resid 222 and name CA)	14.97	1.10	1.11
	assign (segid 3A4 and resid 141 and name CB)	(segid 3A4 and resid 222 and name CB)	14.56	1.13	1.13
	assign (segid 3A4 and resid 141 and name CB)	(segid 3A4 and resid 223 and name CA)	17.81	0.81	0.81
	assign (segid 3A4 and resid 141 and name CB)	(segid 3A4 and resid 223 and name CB)	17.88	0.70	0.71
45	assign (segid 3A4 and resid 141 and name CB)	(segid 3A4 and resid 224 and name CA)	18.14	0.78	0.78
	assign (segid 3A4 and resid 141 and name CB)	(segid 3A4 and resid 245 and name CA)	17.81	0.62	0.61
	assign (segid 3A4 and resid 141 and name CB)	(segid 3A4 and resid 245 and name CB)	18.27	0.75	0.75
	assign (segid 3A4 and resid 141 and name CB)	(segid 3A4 and resid 247 and name CA)	19.23	0.31	0.31
	assign (segid 3A4 and resid 141 and name CB)	(segid 3A4 and resid 247 and name CB)	19.47	0.34	0.34
50	assign (segid 3A4 and resid 141 and name CB)	(segid 3A4 and resid 248 and name CA)	15.47	0.33	0.33
	assign (segid 3A4 and resid 141 and name CB)	(segid 3A4 and resid 248 and name CB)	14.63	0.42	0.42
	assign (segid 3A4 and resid 141 and name CB)	(segid 3A4 and resid 249 and name CA)	16.47	0.33	0.33
	assign (segid 3A4 and resid 141 and name CB)	(segid 3A4 and resid 250 and name CA)	18.89	0.30	0.31
	assign (segid 3A4 and resid 141 and name CB)	(segid 3A4 and resid 251 and name CA)	16.72	0.44	0.45
55	assign (segid 3A4 and resid 141 and name CB)	(segid 3A4 and resid 251 and name CB)	16.06	0.41	0.42
	assign (segid 3A4 and resid 141 and name CB)	(segid 3A4 and resid 252 and name CA)	14.41	0.61	0.60
	assign (segid 3A4 and resid 141 and name CB)	(segid 3A4 and resid 252 and name CB)	13.70	0.51	0.51
	assign (segid 3A4 and resid 141 and name CB)	(segid 3A4 and resid 253 and name CA)	17.47	0.67	0.68
	assign (segid 3A4 and resid 141 and name CB)	(segid 3A4 and resid 256 and name CA)	16.34	1.52	1.52
60	assign (segid 3A4 and resid 141 and name CB)	(segid 3A4 and resid 141 and name C)	2.45	0.05	0.05
	assign (segid 3A4 and resid 141 and name N)	(segid 3A4 and resid 141 and name CA)	1.47	0.01	0.00
	assign (segid 3A4 and resid 141 and name N)	(segid 3A4 and resid 141 and name CB)	2.39	0.05	0.05
	assign (segid 3A4 and resid 141 and name N)	(segid 3A4 and resid 141 and name O)	2.79	0.11	0.11
	assign (segid 3A4 and resid 141 and name N)	(segid 3A4 and resid 141 and name CB)	3.17	0.13	0.14
65	assign (segid 3A4 and resid 141 and name O)	(segid 3A4 and resid 141 and name CB)	2.49	0.05	0.04
	assign (segid 3A4 and resid 147 and name C)	(segid 3A4 and resid 147 and name O)	1.24	0.01	0.01
	assign (segid 3A4 and resid 147 and name C)	(segid 3A4 and resid 148 and name C)	3.07	0.07	0.07
	assign (segid 3A4 and resid 147 and name C)	(segid 3A4 and resid 148 and name CA)	2.46	0.02	0.01
	assign (segid 3A4 and resid 147 and name C)	(segid 3A4 and resid 148 and name N)	1.33	0.01	0.01
70	assign (segid 3A4 and resid 147 and name C)	(segid 3A4 and resid 148 and name O)	4.06	0.16	0.16
	assign (segid 3A4 and resid 147 and name C)	(segid 3A4 and resid 149 and name C)	4.64	0.14	0.15
	assign (segid 3A4 and resid 147 and name C)	(segid 3A4 and resid 149 and name CA)	4.39	0.06	0.07
	assign (segid 3A4 and resid 147 and name C)	(segid 3A4 and resid 149 and name CB)	5.09	0.15	0.16
	assign (segid 3A4 and resid 147 and name C)	(segid 3A4 and resid 149 and name N)	3.15	0.07	0.06
75	assign (segid 3A4 and resid 147 and name C)	(segid 3A4 and resid 149 and name O)	5.79	0.22	0.22
	assign (segid 3A4 and resid 147 and name C)	(segid 3A4 and resid 150 and name C)	5.61	0.52	0.51
	assign (segid 3A4 and resid 147 and name C)	(segid 3A4 and resid 150 and name CA)	4.77	0.20	0.20
	assign (segid 3A4 and resid 147 and name C)	(segid 3A4 and resid 150 and name N)	3.94	0.13	0.12
	assign (segid 3A4 and resid 147 and name C)	(segid 3A4 and resid 150 and name O)	6.51	0.62	0.63
80	assign (segid 3A4 and resid 147 and name C)	(segid 3A4 and resid 151 and name N)	5.61	0.94	0.94
	assign (segid 3A4 and resid 147 and name C)	(segid 3A4 and resid 147 and name C)	1.52	0.01	0.01
	assign (segid 3A4 and resid 147 and name CA)	(segid 3A4 and resid 147 and name CB)	1.52	0.02	0.02

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	assign (segid 3A4 and resid 147 and name CA) (segid 3A4 and resid 147 and name O)	2.40	0.01	0.01
	assign (segid 3A4 and resid 147 and name CA) (segid 3A4 and resid 148 and name C)	4.45	0.05	0.06
	assign (segid 3A4 and resid 147 and name CA) (segid 3A4 and resid 148 and name CA)	3.82	0.03	0.02
	assign (segid 3A4 and resid 147 and name CA) (segid 3A4 and resid 148 and name N)	2.43	0.04	0.04
	assign (segid 3A4 and resid 147 and name CA) (segid 3A4 and resid 148 and name O)	5.47	0.15	0.16
5	assign (segid 3A4 and resid 147 and name CA) (segid 3A4 and resid 149 and name C)	5.62	0.18	0.17
	assign (segid 3A4 and resid 147 and name CA) (segid 3A4 and resid 149 and name CA)	5.44	0.08	0.08
	assign (segid 3A4 and resid 147 and name CA) (segid 3A4 and resid 149 and name CB)	5.83	0.11	0.12
	assign (segid 3A4 and resid 147 and name CA) (segid 3A4 and resid 149 and name N)	4.30	0.08	0.08
	assign (segid 3A4 and resid 147 and name CA) (segid 3A4 and resid 149 and name O)	6.76	0.20	0.21
10	assign (segid 3A4 and resid 147 and name CA) (segid 3A4 and resid 150 and name C)	6.47	0.58	0.57
	assign (segid 3A4 and resid 147 and name CA) (segid 3A4 and resid 150 and name CA)	5.44	0.31	0.31
	assign (segid 3A4 and resid 147 and name CA) (segid 3A4 and resid 150 and name N)	4.78	0.23	0.24
	assign (segid 3A4 and resid 147 and name CA) (segid 3A4 and resid 151 and name CA)	7.84	1.03	1.04
	assign (segid 3A4 and resid 147 and name CA) (segid 3A4 and resid 151 and name N)	6.64	0.93	0.92
15	assign (segid 3A4 and resid 147 and name CA) (segid 3A4 and resid 152 and name CA)	9.77	0.70	0.70
	assign (segid 3A4 and resid 147 and name CA) (segid 3A4 and resid 152 and name CB)	9.68	0.65	0.65
	assign (segid 3A4 and resid 147 and name CA) (segid 3A4 and resid 153 and name CA)	10.33	0.58	0.58
	assign (segid 3A4 and resid 147 and name CA) (segid 3A4 and resid 153 and name CB)	9.64	0.73	0.73
	assign (segid 3A4 and resid 147 and name CA) (segid 3A4 and resid 154 and name CA)	11.25	0.71	0.70
20	assign (segid 3A4 and resid 147 and name CA) (segid 3A4 and resid 155 and name CA)	13.71	0.92	0.91
	assign (segid 3A4 and resid 147 and name CA) (segid 3A4 and resid 155 and name CB)	13.60	1.04	1.04
	assign (segid 3A4 and resid 147 and name CA) (segid 3A4 and resid 156 and name CA)	15.10	0.64	0.64
	assign (segid 3A4 and resid 147 and name CA) (segid 3A4 and resid 156 and name CB)	14.54	0.61	0.61
	assign (segid 3A4 and resid 147 and name CA) (segid 3A4 and resid 157 and name CA)	15.72	0.63	0.64
25	assign (segid 3A4 and resid 147 and name CA) (segid 3A4 and resid 157 and name CB)	14.83	0.65	0.64
	assign (segid 3A4 and resid 147 and name CA) (segid 3A4 and resid 158 and name CA)	17.28	0.85	0.84
	assign (segid 3A4 and resid 147 and name CA) (segid 3A4 and resid 158 and name CB)	16.75	0.96	0.96
	assign (segid 3A4 and resid 147 and name CA) (segid 3A4 and resid 158 and name N)	15.55	3.13	3.13
	assign (segid 3A4 and resid 147 and name CA) (segid 3A4 and resid 193 and name CA)	15.01	3.51	3.51
30	assign (segid 3A4 and resid 147 and name CA) (segid 3A4 and resid 193 and name CB)	14.47	2.06	2.07
	assign (segid 3A4 and resid 147 and name CA) (segid 3A4 and resid 194 and name CA)	14.88	1.92	1.91
	assign (segid 3A4 and resid 147 and name CA) (segid 3A4 and resid 194 and name CB)	17.06	1.74	1.74
	assign (segid 3A4 and resid 147 and name CA) (segid 3A4 and resid 195 and name CA)	16.39	1.86	1.86
	assign (segid 3A4 and resid 147 and name CA) (segid 3A4 and resid 196 and name CA)	16.43	2.20	2.20
35	assign (segid 3A4 and resid 147 and name CA) (segid 3A4 and resid 196 and name CB)	13.12	1.29	1.29
	assign (segid 3A4 and resid 147 and name CA) (segid 3A4 and resid 197 and name CA)	12.18	1.41	1.42
	assign (segid 3A4 and resid 147 and name CA) (segid 3A4 and resid 197 and name CB)	14.51	0.70	0.70
	assign (segid 3A4 and resid 147 and name CA) (segid 3A4 and resid 198 and name CA)	15.17	0.87	0.87
	assign (segid 3A4 and resid 147 and name CA) (segid 3A4 and resid 198 and name CB)	17.31	0.73	0.74
40	assign (segid 3A4 and resid 147 and name CA) (segid 3A4 and resid 199 and name CA)	18.16	0.97	0.98
	assign (segid 3A4 and resid 147 and name CA) (segid 3A4 and resid 199 and name CB)	15.79	0.75	0.74
	assign (segid 3A4 and resid 147 and name CA) (segid 3A4 and resid 201 and name CA)	14.38	1.08	1.08
	assign (segid 3A4 and resid 147 and name CA) (segid 3A4 and resid 201 and name CB)	13.57	1.05	1.05
	assign (segid 3A4 and resid 147 and name CA) (segid 3A4 and resid 202 and name CA)	17.62	1.09	1.09
45	assign (segid 3A4 and resid 147 and name CA) (segid 3A4 and resid 204 and name CA)	17.44	1.68	1.69
	assign (segid 3A4 and resid 147 and name CA) (segid 3A4 and resid 204 and name CB)	16.08	1.75	1.75
	assign (segid 3A4 and resid 147 and name CA) (segid 3A4 and resid 248 and name CB)	16.73	1.08	1.07
	assign (segid 3A4 and resid 147 and name CA) (segid 3A4 and resid 249 and name CA)	17.10	1.23	1.23
50	assign (segid 3A4 and resid 147 and name CA) (segid 3A4 and resid 252 and name CA)	14.85	1.20	1.20
	assign (segid 3A4 and resid 147 and name CA) (segid 3A4 and resid 252 and name CB)	14.06	1.10	1.10
	assign (segid 3A4 and resid 147 and name CA) (segid 3A4 and resid 253 and name CA)	16.86	1.23	1.23
	assign (segid 3A4 and resid 147 and name CA) (segid 3A4 and resid 256 and name CA)	15.78	1.56	1.56
	assign (segid 3A4 and resid 147 and name CA) (segid 3A4 and resid 260 and name CA)	18.66	1.18	1.18
	assign (segid 3A4 and resid 147 and name CA) (segid 3A4 and resid 260 and name CB)	17.76	1.22	1.21
55	assign (segid 3A4 and resid 147 and name CA) (segid 3A4 and resid 260 and name N)	5.45	0.08	0.07
	assign (segid 3A4 and resid 147 and name CB) (segid 3A4 and resid 148 and name CA)	4.48	0.13	0.13
	assign (segid 3A4 and resid 147 and name CB) (segid 3A4 and resid 148 and name N)	3.14	0.14	0.13
	assign (segid 3A4 and resid 147 and name CB) (segid 3A4 and resid 148 and name O)	6.40	0.12	0.11
	assign (segid 3A4 and resid 147 and name CB) (segid 3A4 and resid 149 and name C)	6.96	0.15	0.16
60	assign (segid 3A4 and resid 147 and name CB) (segid 3A4 and resid 149 and name CA)	6.78	0.07	0.06
	assign (segid 3A4 and resid 147 and name CB) (segid 3A4 and resid 149 and name CB)	7.25	0.12	0.13
	assign (segid 3A4 and resid 147 and name CB) (segid 3A4 and resid 149 and name N)	5.54	0.08	0.08
	assign (segid 3A4 and resid 147 and name CB) (segid 3A4 and resid 150 and name CA)	6.64	0.28	0.28
	assign (segid 3A4 and resid 147 and name CB) (segid 3A4 and resid 150 and name N)	6.09	0.19	0.19
65	assign (segid 3A4 and resid 147 and name CB) (segid 3A4 and resid 151 and name CA)	8.71	1.10	1.09
	assign (segid 3A4 and resid 147 and name CB) (segid 3A4 and resid 152 and name CA)	10.91	0.77	0.76
	assign (segid 3A4 and resid 147 and name CB) (segid 3A4 and resid 152 and name CB)	10.87	0.69	0.70
	assign (segid 3A4 and resid 147 and name CB) (segid 3A4 and resid 153 and name CA)	11.63	0.60	0.60
	assign (segid 3A4 and resid 147 and name CB) (segid 3A4 and resid 153 and name CB)	11.00	0.76	0.75
70	assign (segid 3A4 and resid 147 and name CB) (segid 3A4 and resid 154 and name CA)	12.27	0.79	0.79
	assign (segid 3A4 and resid 147 and name CB) (segid 3A4 and resid 155 and name CA)	14.69	1.03	1.03
	assign (segid 3A4 and resid 147 and name CB) (segid 3A4 and resid 155 and name CB)	14.56	1.16	1.15
	assign (segid 3A4 and resid 147 and name CB) (segid 3A4 and resid 156 and name CA)	16.30	0.71	0.71
	assign (segid 3A4 and resid 147 and name CB) (segid 3A4 and resid 156 and name CB)	15.81	0.65	0.65
75	assign (segid 3A4 and resid 147 and name CB) (segid 3A4 and resid 157 and name CA)	16.88	0.72	0.73
	assign (segid 3A4 and resid 147 and name CB) (segid 3A4 and resid 157 and name CB)	15.97	0.75	0.75
	assign (segid 3A4 and resid 147 and name CB) (segid 3A4 and resid 194 and name CA)	15.59	2.43	2.44
	assign (segid 3A4 and resid 147 and name CB) (segid 3A4 and resid 194 and name CB)	16.01	2.23	2.22
	assign (segid 3A4 and resid 147 and name CB) (segid 3A4 and resid 196 and name CA)	17.30	2.44	2.44
80	assign (segid 3A4 and resid 147 and name CB) (segid 3A4 and resid 197 and name CA)	14.11	1.79	1.78
	assign (segid 3A4 and resid 147 and name CB) (segid 3A4 and resid 197 and name CB)	13.23	1.88	1.88
	assign (segid 3A4 and resid 147 and name CB) (segid 3A4 and resid 198 and name CA)	15.58	0.98	0.98

	assign (segid 3A4 and resid 147 and name CB)	(segid 3A4 and resid 198 and name CB)	16.28	1.10	1.10
	assign (segid 3A4 and resid 147 and name CB)	(segid 3A4 and resid 199 and name CA)	18.25	1.11	1.12
	assign (segid 3A4 and resid 147 and name CB)	(segid 3A4 and resid 200 and name CA)	16.59	1.05	1.05
	assign (segid 3A4 and resid 147 and name CB)	(segid 3A4 and resid 201 and name CA)	15.26	0.83	0.83
5	assign (segid 3A4 and resid 147 and name CB)	(segid 3A4 and resid 201 and name CB)	14.53	0.75	0.76
	assign (segid 3A4 and resid 147 and name CB)	(segid 3A4 and resid 204 and name CA)	18.04	1.45	1.45
	assign (segid 3A4 and resid 147 and name CB)	(segid 3A4 and resid 204 and name CB)	16.68	1.50	1.50
	assign (segid 3A4 and resid 147 and name CB)	(segid 3A4 and resid 252 and name CA)	16.07	1.22	1.22
	assign (segid 3A4 and resid 147 and name CB)	(segid 3A4 and resid 252 and name CB)	15.31	1.08	1.08
10	assign (segid 3A4 and resid 147 and name CB)	(segid 3A4 and resid 256 and name CA)	16.86	1.73	1.73
	assign (segid 3A4 and resid 147 and name N)	(segid 3A4 and resid 147 and name C)	2.52	0.03	0.02
	assign (segid 3A4 and resid 147 and name N)	(segid 3A4 and resid 147 and name CA)	1.46	0.00	0.01
	assign (segid 3A4 and resid 147 and name N)	(segid 3A4 and resid 147 and name CB)	2.43	0.05	0.05
	assign (segid 3A4 and resid 147 and name N)	(segid 3A4 and resid 147 and name O)	3.54	0.05	0.05
15	assign (segid 3A4 and resid 147 and name N)	(segid 3A4 and resid 148 and name CA)	4.84	0.06	0.06
	assign (segid 3A4 and resid 147 and name N)	(segid 3A4 and resid 148 and name N)	4.30	0.09	0.10
	assign (segid 3A4 and resid 147 and name N)	(segid 3A4 and resid 148 and name O)	2.90	0.10	0.10
	assign (segid 3A4 and resid 147 and name N)	(segid 3A4 and resid 148 and name O)	5.91	0.21	0.20
20	assign (segid 3A4 and resid 147 and name N)	(segid 3A4 and resid 149 and name C)	5.96	0.18	0.17
	assign (segid 3A4 and resid 147 and name N)	(segid 3A4 and resid 149 and name CB)	5.55	0.12	0.11
	assign (segid 3A4 and resid 147 and name N)	(segid 3A4 and resid 149 and name N)	5.57	0.13	0.13
	assign (segid 3A4 and resid 147 and name N)	(segid 3A4 and resid 149 and name O)	4.49	0.16	0.15
	assign (segid 3A4 and resid 147 and name N)	(segid 3A4 and resid 149 and name O)	7.12	0.17	0.17
25	assign (segid 3A4 and resid 147 and name N)	(segid 3A4 and resid 150 and name CA)	6.11	0.35	0.36
	assign (segid 3A4 and resid 147 and name O)	(segid 3A4 and resid 150 and name N)	5.29	0.30	0.29
	assign (segid 3A4 and resid 147 and name O)	(segid 3A4 and resid 147 and name CB)	3.28	0.09	0.08
	assign (segid 3A4 and resid 147 and name O)	(segid 3A4 and resid 148 and name C)	3.05	0.11	0.10
	assign (segid 3A4 and resid 147 and name O)	(segid 3A4 and resid 148 and name CA)	2.80	0.04	0.04
30	assign (segid 3A4 and resid 147 and name O)	(segid 3A4 and resid 148 and name N)	2.25	0.01	0.02
	assign (segid 3A4 and resid 147 and name O)	(segid 3A4 and resid 148 and name O)	3.82	0.31	0.31
	assign (segid 3A4 and resid 147 and name O)	(segid 3A4 and resid 149 and name C)	4.07	0.18	0.18
	assign (segid 3A4 and resid 147 and name O)	(segid 3A4 and resid 149 and name CA)	4.17	0.16	0.17
	assign (segid 3A4 and resid 147 and name O)	(segid 3A4 and resid 149 and name CB)	5.12	0.26	0.26
	assign (segid 3A4 and resid 147 and name O)	(segid 3A4 and resid 149 and name N)	3.13	0.19	0.19
35	assign (segid 3A4 and resid 147 and name O)	(segid 3A4 and resid 149 and name O)	5.12	0.27	0.28
	assign (segid 3A4 and resid 147 and name O)	(segid 3A4 and resid 150 and name C)	4.54	0.54	0.54
	assign (segid 3A4 and resid 147 and name O)	(segid 3A4 and resid 150 and name CA)	3.85	0.15	0.15
	assign (segid 3A4 and resid 147 and name O)	(segid 3A4 and resid 150 and name N)	3.22	0.09	0.09
	assign (segid 3A4 and resid 147 and name O)	(segid 3A4 and resid 150 and name O)	5.43	0.69	0.69
40	assign (segid 3A4 and resid 147 and name O)	(segid 3A4 and resid 151 and name CA)	5.63	1.09	1.09
	assign (segid 3A4 and resid 147 and name O)	(segid 3A4 and resid 151 and name N)	4.50	0.97	0.98
	assign (segid 3A4 and resid 147 and name O)	(segid 3A4 and resid 152 and name N)	6.50	0.90	0.90
	assign (segid 3A4 and resid 148 and name C)	(segid 3A4 and resid 148 and name O)	1.23	0.00	0.00
	assign (segid 3A4 and resid 148 and name C)	(segid 3A4 and resid 149 and name C)	3.28	0.19	0.20
45	assign (segid 3A4 and resid 148 and name C)	(segid 3A4 and resid 149 and name CA)	2.43	0.01	0.02
	assign (segid 3A4 and resid 148 and name C)	(segid 3A4 and resid 149 and name CB)	3.53	0.21	0.21
	assign (segid 3A4 and resid 148 and name C)	(segid 3A4 and resid 149 and name N)	1.33	0.00	0.01
	assign (segid 3A4 and resid 148 and name C)	(segid 3A4 and resid 149 and name O)	4.25	0.30	0.30
50	assign (segid 3A4 and resid 148 and name C)	(segid 3A4 and resid 150 and name C)	5.20	0.41	0.40
	assign (segid 3A4 and resid 148 and name C)	(segid 3A4 and resid 150 and name CA)	4.75	0.25	0.25
	assign (segid 3A4 and resid 148 and name C)	(segid 3A4 and resid 150 and name N)	3.47	0.21	0.20
	assign (segid 3A4 and resid 148 and name C)	(segid 3A4 and resid 150 and name O)	6.05	0.42	0.42
	assign (segid 3A4 and resid 148 and name C)	(segid 3A4 and resid 151 and name N)	4.99	0.96	0.95
55	assign (segid 3A4 and resid 148 and name C)	(segid 3A4 and resid 152 and name CB)	6.12	0.91	0.91
	assign (segid 3A4 and resid 148 and name CA)	(segid 3A4 and resid 152 and name N)	5.70	1.03	1.03
	assign (segid 3A4 and resid 148 and name CA)	(segid 3A4 and resid 148 and name C)	1.52	0.01	0.01
	assign (segid 3A4 and resid 148 and name CA)	(segid 3A4 and resid 148 and name O)	2.38	0.02	0.02
	assign (segid 3A4 and resid 148 and name CA)	(segid 3A4 and resid 149 and name C)	4.59	0.12	0.12
60	assign (segid 3A4 and resid 148 and name CA)	(segid 3A4 and resid 149 and name CA)	3.81	0.01	0.01
	assign (segid 3A4 and resid 148 and name CA)	(segid 3A4 and resid 149 and name CB)	4.75	0.14	0.13
	assign (segid 3A4 and resid 148 and name CA)	(segid 3A4 and resid 149 and name N)	2.44	0.02	0.02
	assign (segid 3A4 and resid 148 and name CA)	(segid 3A4 and resid 149 and name O)	5.62	0.24	0.25
	assign (segid 3A4 and resid 148 and name CA)	(segid 3A4 and resid 150 and name C)	6.14	0.37	0.37
	assign (segid 3A4 and resid 148 and name CA)	(segid 3A4 and resid 150 and name CA)	5.65	0.16	0.16
65	assign (segid 3A4 and resid 148 and name CA)	(segid 3A4 and resid 150 and name N)	4.49	0.13	0.13
	assign (segid 3A4 and resid 148 and name CA)	(segid 3A4 and resid 150 and name O)	7.01	0.58	0.58
	assign (segid 3A4 and resid 148 and name CA)	(segid 3A4 and resid 151 and name CA)	6.74	1.06	1.05
	assign (segid 3A4 and resid 148 and name CA)	(segid 3A4 and resid 151 and name N)	5.87	0.91	0.92
	assign (segid 3A4 and resid 148 and name CA)	(segid 3A4 and resid 152 and name CA)	7.85	1.00	1.00
70	assign (segid 3A4 and resid 148 and name CA)	(segid 3A4 and resid 152 and name CB)	7.45	0.93	0.93
	assign (segid 3A4 and resid 148 and name CA)	(segid 3A4 and resid 153 and name CA)	9.60	0.66	0.66
	assign (segid 3A4 and resid 148 and name CA)	(segid 3A4 and resid 153 and name CB)	9.32	0.62	0.62
	assign (segid 3A4 and resid 148 and name CA)	(segid 3A4 and resid 154 and name CA)	10.99	0.83	0.83
	assign (segid 3A4 and resid 148 and name CA)	(segid 3A4 and resid 155 and name CA)	12.52	1.17	1.17
75	assign (segid 3A4 and resid 148 and name CA)	(segid 3A4 and resid 155 and name CB)	12.04	1.32	1.33
	assign (segid 3A4 and resid 148 and name CA)	(segid 3A4 and resid 156 and name CA)	13.95	0.93	0.92
	assign (segid 3A4 and resid 148 and name CA)	(segid 3A4 and resid 156 and name CB)	13.36	0.86	0.86
	assign (segid 3A4 and resid 148 and name CA)	(segid 3A4 and resid 157 and name CA)	15.42	0.81	0.81
	assign (segid 3A4 and resid 148 and name CA)	(segid 3A4 and resid 157 and name CB)	14.85	0.80	0.80
80	assign (segid 3A4 and resid 148 and name CA)	(segid 3A4 and resid 158 and name CA)	16.86	1.04	1.04
	assign (segid 3A4 and resid 148 and name CA)	(segid 3A4 and resid 158 and name CB)	16.28	1.13	1.12
	assign (segid 3A4 and resid 148 and name CA)	(segid 3A4 and resid 193 and name CA)	13.71	3.36	3.36
	assign (segid 3A4 and resid 148 and name CA)	(segid 3A4 and resid 193 and name CB)	13.20	3.57	3.56

assign (segid 3A4 and resid 149 and name CA) (segid 3A4 and resid 151 and name N) 4.59 0.41 0.41
 assign (segid 3A4 and resid 149 and name CA) (segid 3A4 and resid 151 and name O) 6.91 0.40 0.39
 assign (segid 3A4 and resid 149 and name CA) (segid 3A4 and resid 152 and name C) 6.09 0.39 0.40
 assign (segid 3A4 and resid 149 and name CA) (segid 3A4 and resid 152 and name CA) 5.50 0.36 0.37
 assign (segid 3A4 and resid 149 and name CA) (segid 3A4 and resid 152 and name CB) 4.90 0.38 0.37
 5 assign (segid 3A4 and resid 149 and name CA) (segid 3A4 and resid 152 and name N) 4.89 0.38 0.38
 assign (segid 3A4 and resid 149 and name CA) (segid 3A4 and resid 153 and name CA) 6.47 0.45 0.45
 assign (segid 3A4 and resid 149 and name CA) (segid 3A4 and resid 153 and name CB) 6.06 0.51 0.51
 assign (segid 3A4 and resid 149 and name CA) (segid 3A4 and resid 153 and name N) 5.51 0.42 0.41
 10 assign (segid 3A4 and resid 149 and name CA) (segid 3A4 and resid 154 and name CA) 8.73 0.43 0.43
 assign (segid 3A4 and resid 149 and name CA) (segid 3A4 and resid 155 and name CA) 10.38 0.57 0.57
 assign (segid 3A4 and resid 149 and name CA) (segid 3A4 and resid 155 and name CB) 10.08 0.69 0.70
 assign (segid 3A4 and resid 149 and name CA) (segid 3A4 and resid 156 and name CA) 11.08 0.43 0.44
 assign (segid 3A4 and resid 149 and name CA) (segid 3A4 and resid 156 and name CB) 10.29 0.42 0.42
 15 assign (segid 3A4 and resid 149 and name CA) (segid 3A4 and resid 157 and name CA) 12.55 0.43 0.42
 assign (segid 3A4 and resid 149 and name CA) (segid 3A4 and resid 157 and name CB) 12.02 0.45 0.46
 assign (segid 3A4 and resid 149 and name CA) (segid 3A4 and resid 158 and name CA) 14.52 0.57 0.57
 assign (segid 3A4 and resid 149 and name CA) (segid 3A4 and resid 158 and name CB) 14.20 0.65 0.66
 assign (segid 3A4 and resid 149 and name CA) (segid 3A4 and resid 159 and name CA) 15.86 0.71 0.70
 20 assign (segid 3A4 and resid 149 and name CA) (segid 3A4 and resid 159 and name CB) 15.29 0.73 0.74
 assign (segid 3A4 and resid 149 and name CA) (segid 3A4 and resid 160 and name CA) 16.95 0.63 0.64
 assign (segid 3A4 and resid 149 and name CA) (segid 3A4 and resid 160 and name CB) 16.24 0.65 0.65
 assign (segid 3A4 and resid 149 and name CA) (segid 3A4 and resid 161 and name CA) 18.62 0.79 0.78
 assign (segid 3A4 and resid 149 and name CA) (segid 3A4 and resid 161 and name CB) 18.15 0.86 0.85
 25 assign (segid 3A4 and resid 149 and name CA) (segid 3A4 and resid 189 and name CA) 17.09 1.66 1.65
 assign (segid 3A4 and resid 149 and name CA) (segid 3A4 and resid 190 and name CA) 14.06 1.76 1.77
 assign (segid 3A4 and resid 149 and name CA) (segid 3A4 and resid 190 and name CB) 14.15 1.88 1.87
 assign (segid 3A4 and resid 149 and name CA) (segid 3A4 and resid 191 and name CA) 15.10 1.46 1.45
 assign (segid 3A4 and resid 149 and name CA) (segid 3A4 and resid 191 and name CB) 16.51 1.44 1.45
 30 assign (segid 3A4 and resid 149 and name CA) (segid 3A4 and resid 192 and name CA) 15.46 1.19 1.18
 assign (segid 3A4 and resid 149 and name CA) (segid 3A4 and resid 192 and name CB) 16.45 1.25 1.25
 assign (segid 3A4 and resid 149 and name CA) (segid 3A4 and resid 193 and name CA) 12.10 1.18 1.18
 assign (segid 3A4 and resid 149 and name CA) (segid 3A4 and resid 193 and name CB) 11.58 1.41 1.42
 assign (segid 3A4 and resid 149 and name CA) (segid 3A4 and resid 194 and name CA) 10.76 0.94 0.94
 35 assign (segid 3A4 and resid 149 and name CA) (segid 3A4 and resid 194 and name CB) 11.15 1.03 1.04
 assign (segid 3A4 and resid 149 and name CA) (segid 3A4 and resid 195 and name CA) 13.63 0.69 0.70
 assign (segid 3A4 and resid 149 and name CA) (segid 3A4 and resid 195 and name CB) 15.02 0.76 0.76
 assign (segid 3A4 and resid 149 and name CA) (segid 3A4 and resid 196 and name CA) 13.13 0.71 0.71
 assign (segid 3A4 and resid 149 and name CA) (segid 3A4 and resid 196 and name CB) 13.20 0.80 0.81
 40 assign (segid 3A4 and resid 149 and name CA) (segid 3A4 and resid 197 and name CA) 9.84 0.78 0.77
 assign (segid 3A4 and resid 149 and name CA) (segid 3A4 and resid 197 and name CB) 8.72 0.64 0.65
 assign (segid 3A4 and resid 149 and name CA) (segid 3A4 and resid 198 and name CA) 11.49 0.53 0.53
 assign (segid 3A4 and resid 149 and name CA) (segid 3A4 and resid 198 and name CB) 12.08 0.43 0.43
 assign (segid 3A4 and resid 149 and name CA) (segid 3A4 and resid 199 and name CA) 14.52 0.77 0.78
 45 assign (segid 3A4 and resid 149 and name CA) (segid 3A4 and resid 199 and name CB) 15.26 0.72 0.73
 assign (segid 3A4 and resid 149 and name CA) (segid 3A4 and resid 200 and name CA) 13.44 1.41 1.42
 assign (segid 3A4 and resid 149 and name CA) (segid 3A4 and resid 201 and name CA) 12.43 1.53 1.52
 assign (segid 3A4 and resid 149 and name CA) (segid 3A4 and resid 201 and name CB) 11.48 1.36 1.36
 50 assign (segid 3A4 and resid 149 and name CA) (segid 3A4 and resid 202 and name CA) 15.72 1.25 1.24
 assign (segid 3A4 and resid 149 and name CA) (segid 3A4 and resid 202 and name CB) 16.24 1.03 1.03
 assign (segid 3A4 and resid 149 and name CA) (segid 3A4 and resid 204 and name CA) 15.07 2.08 2.09
 assign (segid 3A4 and resid 149 and name CA) (segid 3A4 and resid 204 and name CB) 15.63 1.26 1.26
 assign (segid 3A4 and resid 149 and name CA) (segid 3A4 and resid 219 and name CA) 16.99 1.18 1.18
 55 assign (segid 3A4 and resid 149 and name CA) (segid 3A4 and resid 219 and name CB) 15.63 1.26 1.26
 assign (segid 3A4 and resid 149 and name CA) (segid 3A4 and resid 220 and name CA) 17.44 0.83 0.83
 assign (segid 3A4 and resid 149 and name CA) (segid 3A4 and resid 220 and name CB) 16.92 0.60 0.61
 assign (segid 3A4 and resid 149 and name CA) (segid 3A4 and resid 221 and name CA) 16.40 1.18 1.19
 assign (segid 3A4 and resid 149 and name CA) (segid 3A4 and resid 221 and name CB) 15.14 1.33 1.32
 60 assign (segid 3A4 and resid 149 and name CA) (segid 3A4 and resid 224 and name CA) 19.43 0.29 0.29
 assign (segid 3A4 and resid 149 and name CA) (segid 3A4 and resid 245 and name CA) 16.75 0.64 0.63
 assign (segid 3A4 and resid 149 and name CA) (segid 3A4 and resid 245 and name CB) 16.88 0.66 0.66
 assign (segid 3A4 and resid 149 and name CA) (segid 3A4 and resid 246 and name CA) 18.17 1.19 1.20
 assign (segid 3A4 and resid 149 and name CA) (segid 3A4 and resid 246 and name CB) 14.79 0.85 0.85
 assign (segid 3A4 and resid 149 and name CA) (segid 3A4 and resid 248 and name CA) 14.17 0.70 0.70
 65 assign (segid 3A4 and resid 149 and name CA) (segid 3A4 and resid 248 and name CB) 13.95 1.37 1.37
 assign (segid 3A4 and resid 149 and name CA) (segid 3A4 and resid 250 and name CA) 16.59 1.50 1.50
 assign (segid 3A4 and resid 149 and name CA) (segid 3A4 and resid 251 and name CA) 15.59 1.16 1.16
 assign (segid 3A4 and resid 149 and name CA) (segid 3A4 and resid 251 and name CB) 15.59 0.98 0.98
 assign (segid 3A4 and resid 149 and name CA) (segid 3A4 and resid 252 and name CA) 12.20 1.33 1.32
 70 assign (segid 3A4 and resid 149 and name CA) (segid 3A4 and resid 252 and name CB) 11.14 1.34 1.34
 assign (segid 3A4 and resid 149 and name CA) (segid 3A4 and resid 253 and name CA) 13.88 1.75 1.76
 assign (segid 3A4 and resid 149 and name CA) (segid 3A4 and resid 256 and name CA) 13.69 1.81 1.80
 assign (segid 3A4 and resid 149 and name CA) (segid 3A4 and resid 257 and name CA) 15.86 1.82 1.83
 assign (segid 3A4 and resid 149 and name CA) (segid 3A4 and resid 259 and name CB) 17.88 1.08 1.08
 75 assign (segid 3A4 and resid 149 and name CA) (segid 3A4 and resid 260 and name CA) 17.32 1.45 1.45
 assign (segid 3A4 and resid 149 and name CA) (segid 3A4 and resid 260 and name CB) 16.21 1.62 1.62
 assign (segid 3A4 and resid 149 and name CB) (segid 3A4 and resid 150 and name C) 5.39 0.06 0.07
 assign (segid 3A4 and resid 149 and name CB) (segid 3A4 and resid 150 and name CA) 4.58 0.13 0.13
 assign (segid 3A4 and resid 149 and name CB) (segid 3A4 and resid 150 and name N) 3.29 0.18 0.17
 80 assign (segid 3A4 and resid 149 and name CB) (segid 3A4 and resid 150 and name O) 6.04 0.26 0.26
 assign (segid 3A4 and resid 149 and name CB) (segid 3A4 and resid 151 and name C) 6.90 0.40 0.40
 assign (segid 3A4 and resid 149 and name CB) (segid 3A4 and resid 151 and name CA) 6.88 0.36 0.35
 assign (segid 3A4 and resid 149 and name CB) (segid 3A4 and resid 151 and name N) 5.76 0.34 0.34
 assign (segid 3A4 and resid 149 and name CB) (segid 3A4 and resid 152 and name CA) 6.39 0.44 0.45

	assign (segid 3A4 and resid 149 and name CB)	(segid 3A4 and resid 152 and name CB)	5.65	0.42	0.41
	assign (segid 3A4 and resid 149 and name CB)	(segid 3A4 and resid 152 and name N)	5.97	0.43	0.44
	assign (segid 3A4 and resid 149 and name CB)	(segid 3A4 and resid 153 and name CA)	6.82	0.59	0.59
	assign (segid 3A4 and resid 149 and name CB)	(segid 3A4 and resid 153 and name CB)	6.18	0.66	0.67
	assign (segid 3A4 and resid 149 and name CB)	(segid 3A4 and resid 153 and name N)	6.07	0.52	0.51
5	assign (segid 3A4 and resid 149 and name CB)	(segid 3A4 and resid 154 and name CA)	9.44	0.49	0.49
	assign (segid 3A4 and resid 149 and name CB)	(segid 3A4 and resid 155 and name CA)	11.20	0.67	0.66
	assign (segid 3A4 and resid 149 and name CB)	(segid 3A4 and resid 155 and name CB)	10.97	0.81	0.81
	assign (segid 3A4 and resid 149 and name CB)	(segid 3A4 and resid 156 and name CA)	11.50	0.58	0.57
	assign (segid 3A4 and resid 149 and name CB)	(segid 3A4 and resid 156 and name CB)	10.56	0.55	0.55
10	assign (segid 3A4 and resid 149 and name CB)	(segid 3A4 and resid 157 and name CA)	12.86	0.51	0.51
	assign (segid 3A4 and resid 149 and name CB)	(segid 3A4 and resid 157 and name CB)	12.30	0.48	0.49
	assign (segid 3A4 and resid 149 and name CB)	(segid 3A4 and resid 158 and name CA)	15.13	0.64	0.64
	assign (segid 3A4 and resid 149 and name CB)	(segid 3A4 and resid 158 and name CB)	14.94	0.73	0.73
	assign (segid 3A4 and resid 149 and name CB)	(segid 3A4 and resid 159 and name CA)	16.43	0.80	0.80
15	assign (segid 3A4 and resid 149 and name CB)	(segid 3A4 and resid 159 and name CB)	15.87	0.83	0.83
	assign (segid 3A4 and resid 149 and name CB)	(segid 3A4 and resid 160 and name CA)	17.23	0.76	0.77
	assign (segid 3A4 and resid 149 and name CB)	(segid 3A4 and resid 160 and name CB)	16.41	0.79	0.79
	assign (segid 3A4 and resid 149 and name CB)	(segid 3A4 and resid 161 and name CA)	18.46	0.98	0.99
	assign (segid 3A4 and resid 149 and name CB)	(segid 3A4 and resid 161 and name CB)	17.40	1.12	1.11
20	assign (segid 3A4 and resid 149 and name CB)	(segid 3A4 and resid 189 and name CA)	17.69	1.22	1.22
	assign (segid 3A4 and resid 149 and name CB)	(segid 3A4 and resid 189 and name CB)	14.42	1.26	1.25
	assign (segid 3A4 and resid 149 and name CB)	(segid 3A4 and resid 190 and name CA)	14.55	1.40	1.40
	assign (segid 3A4 and resid 149 and name CB)	(segid 3A4 and resid 190 and name CB)	15.25	0.93	0.93
	assign (segid 3A4 and resid 149 and name CB)	(segid 3A4 and resid 191 and name CA)	16.65	0.94	0.94
25	assign (segid 3A4 and resid 149 and name CB)	(segid 3A4 and resid 191 and name CB)	15.52	0.61	0.61
	assign (segid 3A4 and resid 149 and name CB)	(segid 3A4 and resid 192 and name CA)	16.54	0.64	0.63
	assign (segid 3A4 and resid 149 and name CB)	(segid 3A4 and resid 192 and name CB)	12.22	0.60	0.61
	assign (segid 3A4 and resid 149 and name CB)	(segid 3A4 and resid 193 and name CA)	11.83	0.82	0.81
	assign (segid 3A4 and resid 149 and name CB)	(segid 3A4 and resid 193 and name CB)	10.74	0.53	0.53
30	assign (segid 3A4 and resid 149 and name CB)	(segid 3A4 and resid 194 and name CA)	11.17	0.63	0.63
	assign (segid 3A4 and resid 149 and name CB)	(segid 3A4 and resid 194 and name CB)	13.42	0.63	0.63
	assign (segid 3A4 and resid 149 and name CB)	(segid 3A4 and resid 195 and name CA)	14.83	0.60	0.61
	assign (segid 3A4 and resid 149 and name CB)	(segid 3A4 and resid 195 and name CB)	12.89	0.85	0.84
	assign (segid 3A4 and resid 149 and name CB)	(segid 3A4 and resid 196 and name CA)	13.05	0.79	0.79
35	assign (segid 3A4 and resid 149 and name CB)	(segid 3A4 and resid 196 and name CB)	9.46	1.11	1.12
	assign (segid 3A4 and resid 149 and name CB)	(segid 3A4 and resid 197 and name CA)	8.41	0.90	0.90
	assign (segid 3A4 and resid 149 and name CB)	(segid 3A4 and resid 197 and name CB)	10.93	1.07	1.07
	assign (segid 3A4 and resid 149 and name CB)	(segid 3A4 and resid 198 and name CA)	11.57	0.88	0.87
	assign (segid 3A4 and resid 149 and name CB)	(segid 3A4 and resid 198 and name CB)	13.96	1.31	1.31
40	assign (segid 3A4 and resid 149 and name CB)	(segid 3A4 and resid 199 and name CA)	14.77	1.24	1.24
	assign (segid 3A4 and resid 149 and name CB)	(segid 3A4 and resid 199 and name CB)	12.82	1.90	1.89
	assign (segid 3A4 and resid 149 and name CB)	(segid 3A4 and resid 200 and name CA)	11.62	2.07	2.08
	assign (segid 3A4 and resid 149 and name CB)	(segid 3A4 and resid 201 and name CA)	10.66	1.92	1.92
	assign (segid 3A4 and resid 149 and name CB)	(segid 3A4 and resid 201 and name CB)	14.94	1.84	1.83
45	assign (segid 3A4 and resid 149 and name CB)	(segid 3A4 and resid 202 and name CA)	15.50	1.62	1.62
	assign (segid 3A4 and resid 149 and name CB)	(segid 3A4 and resid 202 and name CB)	14.27	2.60	2.59
	assign (segid 3A4 and resid 149 and name CB)	(segid 3A4 and resid 204 and name CA)	16.19	1.49	1.49
	assign (segid 3A4 and resid 149 and name CB)	(segid 3A4 and resid 219 and name CA)	14.83	1.58	1.58
	assign (segid 3A4 and resid 149 and name CB)	(segid 3A4 and resid 219 and name CB)	16.69	1.26	1.26
50	assign (segid 3A4 and resid 149 and name CB)	(segid 3A4 and resid 220 and name CA)	16.22	1.00	1.01
	assign (segid 3A4 and resid 149 and name CB)	(segid 3A4 and resid 220 and name CB)	15.60	1.77	1.77
	assign (segid 3A4 and resid 149 and name CB)	(segid 3A4 and resid 221 and name CA)	14.32	1.93	1.92
	assign (segid 3A4 and resid 149 and name CB)	(segid 3A4 and resid 221 and name CB)	16.20	0.72	0.73
	assign (segid 3A4 and resid 149 and name CB)	(segid 3A4 and resid 245 and name CA)	16.37	0.72	0.73
55	assign (segid 3A4 and resid 149 and name CB)	(segid 3A4 and resid 245 and name CB)	17.76	0.93	0.92
	assign (segid 3A4 and resid 149 and name CB)	(segid 3A4 and resid 246 and name CA)	17.84	0.86	0.87
	assign (segid 3A4 and resid 149 and name CB)	(segid 3A4 and resid 247 and name CA)	14.23	0.81	0.80
	assign (segid 3A4 and resid 149 and name CB)	(segid 3A4 and resid 248 and name CA)	13.57	0.81	0.81
	assign (segid 3A4 and resid 149 and name CB)	(segid 3A4 and resid 248 and name CB)	13.61	1.10	1.10
60	assign (segid 3A4 and resid 149 and name CB)	(segid 3A4 and resid 249 and name CA)	16.28	1.25	1.26
	assign (segid 3A4 and resid 149 and name CB)	(segid 3A4 and resid 250 and name CA)	17.68	1.20	1.19
	assign (segid 3A4 and resid 149 and name CB)	(segid 3A4 and resid 251 and name CA)	15.18	1.04	1.04
	assign (segid 3A4 and resid 149 and name CB)	(segid 3A4 and resid 251 and name CB)	15.10	0.90	0.89
	assign (segid 3A4 and resid 149 and name CB)	(segid 3A4 and resid 252 and name CA)	11.88	1.23	1.23
65	assign (segid 3A4 and resid 149 and name CB)	(segid 3A4 and resid 252 and name CB)	10.83	1.22	1.21
	assign (segid 3A4 and resid 149 and name CB)	(segid 3A4 and resid 253 and name CA)	13.80	1.59	1.58
	assign (segid 3A4 and resid 149 and name CB)	(segid 3A4 and resid 254 and name CA)	16.84	1.58	1.57
	assign (segid 3A4 and resid 149 and name CB)	(segid 3A4 and resid 254 and name CB)	15.60	1.91	1.91
	assign (segid 3A4 and resid 149 and name CB)	(segid 3A4 and resid 255 and name CA)	13.61	1.89	1.89
70	assign (segid 3A4 and resid 149 and name CB)	(segid 3A4 and resid 256 and name CA)	15.92	1.96	1.97
	assign (segid 3A4 and resid 149 and name CB)	(segid 3A4 and resid 257 and name CA)	17.79	1.33	1.33
	assign (segid 3A4 and resid 149 and name CB)	(segid 3A4 and resid 259 and name CB)	17.40	1.81	1.82
	assign (segid 3A4 and resid 149 and name CB)	(segid 3A4 and resid 260 and name CA)	16.32	1.99	1.98
	assign (segid 3A4 and resid 149 and name CB)	(segid 3A4 and resid 260 and name CB)	2.46	0.03	0.03
75	assign (segid 3A4 and resid 149 and name N)	(segid 3A4 and resid 149 and name C)	1.46	0.00	0.01
	assign (segid 3A4 and resid 149 and name N)	(segid 3A4 and resid 149 and name CB)	2.45	0.03	0.02
	assign (segid 3A4 and resid 149 and name N)	(segid 3A4 and resid 149 and name O)	3.54	0.08	0.09
	assign (segid 3A4 and resid 149 and name N)	(segid 3A4 and resid 150 and name C)	1.83	0.16	0.16
	assign (segid 3A4 and resid 149 and name N)	(segid 3A4 and resid 150 and name CA)	4.16	0.04	0.03
80	assign (segid 3A4 and resid 149 and name N)	(segid 3A4 and resid 150 and name N)	2.74	0.05	0.05
	assign (segid 3A4 and resid 149 and name N)	(segid 3A4 and resid 150 and name O)	5.65	0.57	0.57
	assign (segid 3A4 and resid 149 and name N)	(segid 3A4 and resid 151 and name C)	6.37	0.53	0.52

	assign (segid 3A4 and resid 149 and name N) (segid 3A4 and resid 151 and name CA)	5.97	0.50	0.51
	assign (segid 3A4 and resid 149 and name N) (segid 3A4 and resid 151 and name N)	4.89	0.50	0.49
	assign (segid 3A4 and resid 149 and name N) (segid 3A4 and resid 152 and name C)	7.15	0.46	0.46
	assign (segid 3A4 and resid 149 and name N) (segid 3A4 and resid 152 and name CA)	6.42	0.54	0.53
5	assign (segid 3A4 and resid 149 and name N) (segid 3A4 and resid 152 and name CB)	5.90	0.58	0.57
	assign (segid 3A4 and resid 149 and name N) (segid 3A4 and resid 152 and name N)	5.61	0.54	0.54
	assign (segid 3A4 and resid 149 and name N) (segid 3A4 and resid 153 and name N)	6.64	0.41	0.41
	assign (segid 3A4 and resid 149 and name N) (segid 3A4 and resid 149 and name CB)	3.14	0.16	0.16
	assign (segid 3A4 and resid 149 and name O) (segid 3A4 and resid 150 and name C)	2.87	0.08	0.08
10	assign (segid 3A4 and resid 149 and name O) (segid 3A4 and resid 150 and name CA)	2.79	0.02	0.01
	assign (segid 3A4 and resid 149 and name O) (segid 3A4 and resid 150 and name N)	2.27	0.01	0.00
	assign (segid 3A4 and resid 149 and name O) (segid 3A4 and resid 150 and name O)	3.30	0.15	0.15
	assign (segid 3A4 and resid 149 and name O) (segid 3A4 and resid 151 and name C)	4.02	0.28	0.29
	assign (segid 3A4 and resid 149 and name O) (segid 3A4 and resid 151 and name CA)	4.25	0.26	0.26
15	assign (segid 3A4 and resid 149 and name O) (segid 3A4 and resid 151 and name N)	3.34	0.27	0.26
	assign (segid 3A4 and resid 149 and name O) (segid 3A4 and resid 151 and name O)	4.97	0.31	0.30
	assign (segid 3A4 and resid 149 and name O) (segid 3A4 and resid 152 and name C)	3.98	0.30	0.31
	assign (segid 3A4 and resid 149 and name O) (segid 3A4 and resid 152 and name CA)	3.77	0.23	0.24
	assign (segid 3A4 and resid 149 and name O) (segid 3A4 and resid 152 and name CB)	3.63	0.23	0.23
20	assign (segid 3A4 and resid 149 and name O) (segid 3A4 and resid 152 and name N)	3.22	0.27	0.28
	assign (segid 3A4 and resid 149 and name O) (segid 3A4 and resid 152 and name O)	5.19	0.31	0.32
	assign (segid 3A4 and resid 149 and name O) (segid 3A4 and resid 153 and name C)	5.23	0.43	0.44
	assign (segid 3A4 and resid 149 and name O) (segid 3A4 and resid 153 and name CA)	4.17	0.43	0.43
	assign (segid 3A4 and resid 149 and name O) (segid 3A4 and resid 153 and name CB)	3.91	0.47	0.48
25	assign (segid 3A4 and resid 149 and name O) (segid 3A4 and resid 153 and name N)	3.22	0.37	0.37
	assign (segid 3A4 and resid 149 and name O) (segid 3A4 and resid 153 and name O)	6.39	0.43	0.43
	assign (segid 3A4 and resid 149 and name O) (segid 3A4 and resid 154 and name CA)	6.43	0.41	0.41
	assign (segid 3A4 and resid 150 and name C) (segid 3A4 and resid 150 and name O)	1.24	0.01	0.01
30	assign (segid 3A4 and resid 150 and name C) (segid 3A4 and resid 151 and name C)	3.05	0.06	0.05
	assign (segid 3A4 and resid 150 and name C) (segid 3A4 and resid 151 and name CA)	2.44	0.01	0.01
	assign (segid 3A4 and resid 150 and name C) (segid 3A4 and resid 151 and name N)	1.34	0.01	0.00
	assign (segid 3A4 and resid 150 and name C) (segid 3A4 and resid 151 and name O)	3.90	0.17	0.17
	assign (segid 3A4 and resid 150 and name C) (segid 3A4 and resid 152 and name C)	4.68	0.16	0.15
35	assign (segid 3A4 and resid 150 and name C) (segid 3A4 and resid 152 and name CA)	4.49	0.05	0.05
	assign (segid 3A4 and resid 150 and name C) (segid 3A4 and resid 152 and name CB)	5.18	0.18	0.19
	assign (segid 3A4 and resid 150 and name C) (segid 3A4 and resid 152 and name N)	3.29	0.09	0.09
	assign (segid 3A4 and resid 150 and name C) (segid 3A4 and resid 152 and name O)	5.70	0.17	0.17
	assign (segid 3A4 and resid 150 and name C) (segid 3A4 and resid 153 and name C)	5.11	0.47	0.47
40	assign (segid 3A4 and resid 150 and name C) (segid 3A4 and resid 153 and name CA)	4.84	0.41	0.40
	assign (segid 3A4 and resid 150 and name C) (segid 3A4 and resid 153 and name CB)	4.76	0.49	0.49
	assign (segid 3A4 and resid 150 and name C) (segid 3A4 and resid 153 and name N)	4.06	0.29	0.28
	assign (segid 3A4 and resid 150 and name C) (segid 3A4 and resid 153 and name O)	6.30	0.47	0.47
	assign (segid 3A4 and resid 150 and name C) (segid 3A4 and resid 154 and name C)	6.25	0.54	0.54
45	assign (segid 3A4 and resid 150 and name C) (segid 3A4 and resid 154 and name CA)	5.12	0.51	0.52
	assign (segid 3A4 and resid 150 and name C) (segid 3A4 and resid 154 and name N)	4.31	0.50	0.50
	assign (segid 3A4 and resid 150 and name C) (segid 3A4 and resid 155 and name N)	6.19	0.56	0.55
	assign (segid 3A4 and resid 150 and name CA) (segid 3A4 and resid 150 and name C)	1.53	0.02	0.01
50	assign (segid 3A4 and resid 150 and name CA) (segid 3A4 and resid 151 and name O)	2.40	0.01	0.01
	assign (segid 3A4 and resid 150 and name CA) (segid 3A4 and resid 151 and name C)	4.45	0.04	0.04
	assign (segid 3A4 and resid 150 and name CA) (segid 3A4 and resid 151 and name CA)	3.82	0.02	0.02
	assign (segid 3A4 and resid 150 and name CA) (segid 3A4 and resid 151 and name N)	2.45	0.03	0.02
	assign (segid 3A4 and resid 150 and name CA) (segid 3A4 and resid 151 and name O)	5.34	0.12	0.12
	assign (segid 3A4 and resid 150 and name CA) (segid 3A4 and resid 152 and name C)	5.65	0.14	0.14
55	assign (segid 3A4 and resid 150 and name CA) (segid 3A4 and resid 152 and name CA)	5.54	0.05	0.05
	assign (segid 3A4 and resid 150 and name CA) (segid 3A4 and resid 152 and name CB)	5.93	0.18	0.19
	assign (segid 3A4 and resid 150 and name CA) (segid 3A4 and resid 152 and name N)	4.44	0.06	0.05
	assign (segid 3A4 and resid 150 and name CA) (segid 3A4 and resid 152 and name O)	6.75	0.15	0.14
	assign (segid 3A4 and resid 150 and name CA) (segid 3A4 and resid 153 and name C)	5.87	0.40	0.41
60	assign (segid 3A4 and resid 150 and name CA) (segid 3A4 and resid 153 and name CA)	5.40	0.36	0.37
	assign (segid 3A4 and resid 150 and name CA) (segid 3A4 and resid 153 and name CB)	4.90	0.47	0.47
	assign (segid 3A4 and resid 150 and name CA) (segid 3A4 and resid 153 and name N)	4.80	0.25	0.25
	assign (segid 3A4 and resid 150 and name CA) (segid 3A4 and resid 154 and name CA)	6.16	0.45	0.44
	assign (segid 3A4 and resid 150 and name CA) (segid 3A4 and resid 154 and name N)	5.27	0.43	0.43
65	assign (segid 3A4 and resid 150 and name CA) (segid 3A4 and resid 155 and name CA)	8.81	0.49	0.50
	assign (segid 3A4 and resid 150 and name CA) (segid 3A4 and resid 155 and name CB)	8.95	0.54	0.54
	assign (segid 3A4 and resid 150 and name CA) (segid 3A4 and resid 156 and name CA)	10.15	0.37	0.38
	assign (segid 3A4 and resid 150 and name CA) (segid 3A4 and resid 156 and name CB)	9.72	0.34	0.34
	assign (segid 3A4 and resid 150 and name CA) (segid 3A4 and resid 157 and name CA)	10.68	0.41	0.41
70	assign (segid 3A4 and resid 150 and name CA) (segid 3A4 and resid 157 and name CB)	9.87	0.43	0.42
	assign (segid 3A4 and resid 150 and name CA) (segid 3A4 and resid 158 and name CA)	12.25	0.64	0.63
	assign (segid 3A4 and resid 150 and name CA) (segid 3A4 and resid 158 and name CB)	11.82	0.76	0.77
	assign (segid 3A4 and resid 150 and name CA) (segid 3A4 and resid 159 and name CA)	14.33	0.77	0.78
	assign (segid 3A4 and resid 150 and name CA) (segid 3A4 and resid 159 and name CB)	14.09	0.82	0.81
75	assign (segid 3A4 and resid 150 and name CA) (segid 3A4 and resid 160 and name CA)	15.56	0.57	0.58
	assign (segid 3A4 and resid 150 and name CA) (segid 3A4 and resid 160 and name CB)	14.96	0.50	0.51
	assign (segid 3A4 and resid 150 and name CA) (segid 3A4 and resid 161 and name CA)	16.59	0.67	0.67
	assign (segid 3A4 and resid 150 and name CA) (segid 3A4 and resid 161 and name CB)	15.94	0.68	0.67
	assign (segid 3A4 and resid 150 and name CA) (segid 3A4 and resid 190 and name CA)	13.74	2.24	2.25
80	assign (segid 3A4 and resid 150 and name CA) (segid 3A4 and resid 190 and name CB)	13.50	2.31	2.31
	assign (segid 3A4 and resid 150 and name CA) (segid 3A4 and resid 191 and name CA)	15.12	1.59	1.60
	assign (segid 3A4 and resid 150 and name CA) (segid 3A4 and resid 191 and name CB)	16.46	1.57	1.57
	assign (segid 3A4 and resid 150 and name CA) (segid 3A4 and resid 192 and name CA)	16.13	1.56	1.55

	assign (segid 3A4 and resid 150 and name CA)	(segid 3A4 and resid 192 and name CB)	17.11	1.76	1.75
	assign (segid 3A4 and resid 150 and name CA)	(segid 3A4 and resid 193 and name CA)	12.99	1.56	1.56
	assign (segid 3A4 and resid 150 and name CA)	(segid 3A4 and resid 193 and name CB)	12.24	1.87	1.87
	assign (segid 3A4 and resid 150 and name CA)	(segid 3A4 and resid 194 and name CA)	11.61	0.88	0.88
	assign (segid 3A4 and resid 150 and name CA)	(segid 3A4 and resid 194 and name CB)	11.64	0.85	0.86
5	assign (segid 3A4 and resid 150 and name CA)	(segid 3A4 and resid 195 and name CA)	14.85	0.71	0.72
	assign (segid 3A4 and resid 150 and name CA)	(segid 3A4 and resid 195 and name CB)	16.11	0.81	0.82
	assign (segid 3A4 and resid 150 and name CA)	(segid 3A4 and resid 196 and name CA)	14.96	0.78	0.78
	assign (segid 3A4 and resid 150 and name CA)	(segid 3A4 and resid 196 and name CB)	15.01	0.95	0.94
	assign (segid 3A4 and resid 150 and name CA)	(segid 3A4 and resid 197 and name CA)	11.97	0.77	0.78
10	assign (segid 3A4 and resid 150 and name CA)	(segid 3A4 and resid 197 and name CB)	10.67	0.74	0.75
	assign (segid 3A4 and resid 150 and name CA)	(segid 3A4 and resid 198 and name CA)	13.41	0.78	0.78
	assign (segid 3A4 and resid 150 and name CA)	(segid 3A4 and resid 198 and name CB)	13.70	0.64	0.65
	assign (segid 3A4 and resid 150 and name CA)	(segid 3A4 and resid 199 and name CA)	16.71	0.80	0.80
	assign (segid 3A4 and resid 150 and name CA)	(segid 3A4 and resid 199 and name CB)	17.40	0.69	0.69
15	assign (segid 3A4 and resid 150 and name CA)	(segid 3A4 and resid 200 and name CA)	16.12	1.28	1.28
	assign (segid 3A4 and resid 150 and name CA)	(segid 3A4 and resid 201 and name CA)	14.99	1.75	1.76
	assign (segid 3A4 and resid 150 and name CA)	(segid 3A4 and resid 201 and name CB)	13.89	1.75	1.76
	assign (segid 3A4 and resid 150 and name CA)	(segid 3A4 and resid 245 and name CA)	18.06	0.48	0.48
	assign (segid 3A4 and resid 150 and name CA)	(segid 3A4 and resid 245 and name CB)	18.28	0.46	0.47
20	assign (segid 3A4 and resid 150 and name CA)	(segid 3A4 and resid 248 and name CA)	15.58	0.74	0.74
	assign (segid 3A4 and resid 150 and name CA)	(segid 3A4 and resid 248 and name CB)	15.23	0.79	0.80
	assign (segid 3A4 and resid 150 and name CA)	(segid 3A4 and resid 249 and name CA)	14.34	0.73	0.73
	assign (segid 3A4 and resid 150 and name CA)	(segid 3A4 and resid 250 and name CA)	16.46	0.84	0.85
	assign (segid 3A4 and resid 150 and name CA)	(segid 3A4 and resid 250 and name CB)	17.92	0.83	0.82
25	assign (segid 3A4 and resid 150 and name CA)	(segid 3A4 and resid 251 and name CA)	15.46	0.89	0.89
	assign (segid 3A4 and resid 150 and name CA)	(segid 3A4 and resid 251 and name CB)	15.68	0.93	0.93
	assign (segid 3A4 and resid 150 and name CA)	(segid 3A4 and resid 252 and name CA)	11.88	0.88	0.89
	assign (segid 3A4 and resid 150 and name CA)	(segid 3A4 and resid 252 and name CB)	11.08	0.78	0.78
	assign (segid 3A4 and resid 150 and name CA)	(segid 3A4 and resid 253 and name CA)	12.99	0.97	0.98
30	assign (segid 3A4 and resid 150 and name CA)	(segid 3A4 and resid 254 and name CA)	15.96	1.10	1.09
	assign (segid 3A4 and resid 150 and name CA)	(segid 3A4 and resid 255 and name CA)	14.73	1.62	1.62
	assign (segid 3A4 and resid 150 and name CA)	(segid 3A4 and resid 256 and name CA)	12.15	1.37	1.37
	assign (segid 3A4 and resid 150 and name CA)	(segid 3A4 and resid 257 and name CA)	13.96	1.04	1.04
	assign (segid 3A4 and resid 150 and name CA)	(segid 3A4 and resid 258 and name CA)	17.21	1.00	1.00
35	assign (segid 3A4 and resid 150 and name CA)	(segid 3A4 and resid 258 and name CB)	17.94	1.00	0.99
	assign (segid 3A4 and resid 150 and name CA)	(segid 3A4 and resid 259 and name CA)	16.73	0.79	0.80
	assign (segid 3A4 and resid 150 and name CA)	(segid 3A4 and resid 259 and name CB)	16.14	0.86	0.85
	assign (segid 3A4 and resid 150 and name CA)	(segid 3A4 and resid 260 and name CA)	15.11	0.98	0.98
	assign (segid 3A4 and resid 150 and name CA)	(segid 3A4 and resid 260 and name CB)	13.98	1.06	1.06
40	assign (segid 3A4 and resid 150 and name CA)	(segid 3A4 and resid 261 and name CA)	17.89	1.06	1.06
	assign (segid 3A4 and resid 150 and name CA)	(segid 3A4 and resid 150 and name C)	2.48	0.02	0.02
	assign (segid 3A4 and resid 150 and name N)	(segid 3A4 and resid 150 and name CA)	1.45	0.01	0.01
	assign (segid 3A4 and resid 150 and name N)	(segid 3A4 and resid 150 and name O)	3.38	0.25	0.26
	assign (segid 3A4 and resid 150 and name N)	(segid 3A4 and resid 151 and name C)	4.90	0.18	0.19
45	assign (segid 3A4 and resid 150 and name N)	(segid 3A4 and resid 151 and name CA)	4.38	0.18	0.18
	assign (segid 3A4 and resid 150 and name N)	(segid 3A4 and resid 151 and name N)	3.01	0.24	0.24
	assign (segid 3A4 and resid 150 and name N)	(segid 3A4 and resid 151 and name O)	5.96	0.22	0.23
	assign (segid 3A4 and resid 150 and name N)	(segid 3A4 and resid 152 and name C)	5.89	0.23	0.24
	assign (segid 3A4 and resid 150 and name N)	(segid 3A4 and resid 152 and name CA)	5.55	0.14	0.15
50	assign (segid 3A4 and resid 150 and name N)	(segid 3A4 and resid 152 and name CB)	5.59	0.21	0.21
	assign (segid 3A4 and resid 150 and name N)	(segid 3A4 and resid 152 and name N)	4.54	0.15	0.14
	assign (segid 3A4 and resid 150 and name N)	(segid 3A4 and resid 152 and name O)	7.08	0.23	0.24
	assign (segid 3A4 and resid 150 and name N)	(segid 3A4 and resid 153 and name C)	6.65	0.42	0.42
	assign (segid 3A4 and resid 150 and name N)	(segid 3A4 and resid 153 and name CA)	5.89	0.40	0.39
55	assign (segid 3A4 and resid 150 and name N)	(segid 3A4 and resid 153 and name CB)	5.37	0.49	0.48
	assign (segid 3A4 and resid 150 and name N)	(segid 3A4 and resid 153 and name N)	5.11	0.32	0.31
	assign (segid 3A4 and resid 150 and name N)	(segid 3A4 and resid 154 and name N)	6.22	0.43	0.44
	assign (segid 3A4 and resid 150 and name O)	(segid 3A4 and resid 151 and name C)	3.00	0.11	0.12
60	assign (segid 3A4 and resid 150 and name O)	(segid 3A4 and resid 151 and name CA)	2.77	0.03	0.02
	assign (segid 3A4 and resid 150 and name O)	(segid 3A4 and resid 151 and name N)	2.25	0.02	0.02
	assign (segid 3A4 and resid 150 and name O)	(segid 3A4 and resid 151 and name O)	3.54	0.35	0.36
	assign (segid 3A4 and resid 150 and name O)	(segid 3A4 and resid 152 and name C)	4.30	0.30	0.30
	assign (segid 3A4 and resid 150 and name O)	(segid 3A4 and resid 152 and name CA)	4.36	0.17	0.16
	assign (segid 3A4 and resid 150 and name O)	(segid 3A4 and resid 152 and name CB)	5.21	0.38	0.37
65	assign (segid 3A4 and resid 150 and name O)	(segid 3A4 and resid 152 and name N)	3.35	0.23	0.23
	assign (segid 3A4 and resid 150 and name O)	(segid 3A4 and resid 152 and name O)	5.18	0.35	0.36
	assign (segid 3A4 and resid 150 and name O)	(segid 3A4 and resid 153 and name C)	4.32	0.94	0.95
	assign (segid 3A4 and resid 150 and name O)	(segid 3A4 and resid 153 and name CA)	4.27	0.76	0.77
	assign (segid 3A4 and resid 150 and name O)	(segid 3A4 and resid 153 and name CB)	4.34	0.85	0.86
70	assign (segid 3A4 and resid 150 and name O)	(segid 3A4 and resid 153 and name N)	3.68	0.51	0.52
	assign (segid 3A4 and resid 150 and name O)	(segid 3A4 and resid 154 and name CA)	4.21	1.06	1.05
	assign (segid 3A4 and resid 150 and name O)	(segid 3A4 and resid 154 and name N)	3.43	1.01	1.01
	assign (segid 3A4 and resid 150 and name O)	(segid 3A4 and resid 155 and name N)	5.39	0.93	0.94
	assign (segid 3A4 and resid 150 and name O)	(segid 3A4 and resid 151 and name O)	1.24	0.01	0.00
75	assign (segid 3A4 and resid 151 and name C)	(segid 3A4 and resid 152 and name C)	3.01	0.08	0.08
	assign (segid 3A4 and resid 151 and name C)	(segid 3A4 and resid 152 and name CA)	2.44	0.02	0.01
	assign (segid 3A4 and resid 151 and name C)	(segid 3A4 and resid 152 and name CB)	3.70	0.03	0.02
	assign (segid 3A4 and resid 151 and name C)	(segid 3A4 and resid 152 and name N)	1.33	0.01	0.01
	assign (segid 3A4 and resid 151 and name C)	(segid 3A4 and resid 152 and name O)	3.76	0.15	0.15
80	assign (segid 3A4 and resid 151 and name C)	(segid 3A4 and resid 153 and name C)	4.58	0.13	0.13
	assign (segid 3A4 and resid 151 and name C)	(segid 3A4 and resid 153 and name CA)	4.51	0.11	0.10
	assign (segid 3A4 and resid 151 and name C)	(segid 3A4 and resid 153 and name CB)	5.33	0.12	0.12

5	assign	(segid 3A4 and resid 151 and name C)	(segid 3A4 and resid 153 and name N)	3.34	0.08	0.08
	assign	(segid 3A4 and resid 151 and name C)	(segid 3A4 and resid 153 and name O)	5.67	0.15	0.15
	assign	(segid 3A4 and resid 151 and name C)	(segid 3A4 and resid 154 and name C)	4.93	0.09	0.09
	assign	(segid 3A4 and resid 151 and name C)	(segid 3A4 and resid 154 and name CA)	4.50	0.14	0.13
	assign	(segid 3A4 and resid 151 and name C)	(segid 3A4 and resid 151 and name N)	3.79	0.13	0.13
	assign	(segid 3A4 and resid 151 and name C)	(segid 3A4 and resid 154 and name O)	6.14	0.09	0.09
	assign	(segid 3A4 and resid 151 and name C)	(segid 3A4 and resid 155 and name C)	6.36	0.26	0.26
	assign	(segid 3A4 and resid 151 and name C)	(segid 3A4 and resid 155 and name CA)	5.26	0.30	0.30
	assign	(segid 3A4 and resid 151 and name C)	(segid 3A4 and resid 155 and name CB)	4.92	0.44	0.44
10	assign	(segid 3A4 and resid 151 and name C)	(segid 3A4 and resid 155 and name N)	4.29	0.20	0.20
	assign	(segid 3A4 and resid 151 and name C)	(segid 3A4 and resid 156 and name CA)	7.50	0.20	0.21
	assign	(segid 3A4 and resid 151 and name C)	(segid 3A4 and resid 156 and name CB)	7.48	0.23	0.23
	assign	(segid 3A4 and resid 151 and name C)	(segid 3A4 and resid 156 and name N)	6.23	0.22	0.22
	assign	(segid 3A4 and resid 151 and name CA)	(segid 3A4 and resid 151 and name C)	1.52	0.01	0.01
15	assign	(segid 3A4 and resid 151 and name CA)	(segid 3A4 and resid 151 and name O)	2.39	0.02	0.03
	assign	(segid 3A4 and resid 151 and name CA)	(segid 3A4 and resid 152 and name C)	4.41	0.07	0.06
	assign	(segid 3A4 and resid 151 and name CA)	(segid 3A4 and resid 152 and name CA)	3.80	0.01	0.01
	assign	(segid 3A4 and resid 151 and name CA)	(segid 3A4 and resid 152 and name CB)	4.83	0.04	0.03
	assign	(segid 3A4 and resid 151 and name CA)	(segid 3A4 and resid 152 and name N)	2.42	0.01	0.02
20	assign	(segid 3A4 and resid 151 and name CA)	(segid 3A4 and resid 152 and name O)	5.23	0.15	0.14
	assign	(segid 3A4 and resid 151 and name CA)	(segid 3A4 and resid 153 and name C)	5.55	0.13	0.13
	assign	(segid 3A4 and resid 151 and name CA)	(segid 3A4 and resid 153 and name CA)	5.53	0.11	0.11
	assign	(segid 3A4 and resid 151 and name CA)	(segid 3A4 and resid 153 and name CB)	6.05	0.13	0.13
	assign	(segid 3A4 and resid 151 and name CA)	(segid 3A4 and resid 153 and name N)	4.46	0.07	0.08
25	assign	(segid 3A4 and resid 151 and name CA)	(segid 3A4 and resid 153 and name O)	6.67	0.14	0.14
	assign	(segid 3A4 and resid 151 and name CA)	(segid 3A4 and resid 154 and name C)	5.77	0.12	0.11
	assign	(segid 3A4 and resid 151 and name CA)	(segid 3A4 and resid 154 and name CA)	5.09	0.14	0.14
	assign	(segid 3A4 and resid 151 and name CA)	(segid 3A4 and resid 154 and name N)	4.57	0.13	0.13
	assign	(segid 3A4 and resid 151 and name CA)	(segid 3A4 and resid 154 and name O)	6.93	0.11	0.11
30	assign	(segid 3A4 and resid 151 and name CA)	(segid 3A4 and resid 155 and name CA)	6.41	0.32	0.32
	assign	(segid 3A4 and resid 151 and name CA)	(segid 3A4 and resid 155 and name CB)	6.17	0.46	0.45
	assign	(segid 3A4 and resid 151 and name CA)	(segid 3A4 and resid 155 and name N)	5.35	0.23	0.23
	assign	(segid 3A4 and resid 151 and name CA)	(segid 3A4 and resid 156 and name CA)	8.86	0.19	0.19
	assign	(segid 3A4 and resid 151 and name CA)	(segid 3A4 and resid 156 and name CB)	8.86	0.21	0.21
35	assign	(segid 3A4 and resid 151 and name CA)	(segid 3A4 and resid 157 and name CA)	10.07	0.21	0.21
	assign	(segid 3A4 and resid 151 and name CA)	(segid 3A4 and resid 157 and name CB)	9.64	0.36	0.36
	assign	(segid 3A4 and resid 151 and name CA)	(segid 3A4 and resid 158 and name CA)	10.69	0.32	0.31
	assign	(segid 3A4 and resid 151 and name CA)	(segid 3A4 and resid 158 and name CB)	9.96	0.39	0.38
	assign	(segid 3A4 and resid 151 and name CA)	(segid 3A4 and resid 159 and name CA)	12.39	0.75	0.75
40	assign	(segid 3A4 and resid 151 and name CA)	(segid 3A4 and resid 159 and name CB)	12.03	0.90	0.89
	assign	(segid 3A4 and resid 151 and name CA)	(segid 3A4 and resid 160 and name CA)	14.35	0.77	0.77
	assign	(segid 3A4 and resid 151 and name CA)	(segid 3A4 and resid 160 and name CB)	14.04	0.82	0.81
	assign	(segid 3A4 and resid 151 and name CA)	(segid 3A4 and resid 161 and name CA)	15.50	0.59	0.59
	assign	(segid 3A4 and resid 151 and name CA)	(segid 3A4 and resid 161 and name CB)	14.99	0.57	0.57
45	assign	(segid 3A4 and resid 151 and name CA)	(segid 3A4 and resid 167 and name CA)	15.70	2.93	2.94
	assign	(segid 3A4 and resid 151 and name CA)	(segid 3A4 and resid 168 and name CA)	15.01	3.05	3.05
	assign	(segid 3A4 and resid 151 and name CA)	(segid 3A4 and resid 169 and name CB)	15.03	3.08	3.08
	assign	(segid 3A4 and resid 151 and name CA)	(segid 3A4 and resid 189 and name CA)	11.76	3.00	2.99
	assign	(segid 3A4				

	assign (segid 3A4 and resid 152 and name CA) (segid 3A4 and resid 154 and name N)	4.36	0.12	0.12
	assign (segid 3A4 and resid 152 and name CA) (segid 3A4 and resid 154 and name O)	6.74	0.13	0.13
	assign (segid 3A4 and resid 152 and name CA) (segid 3A4 and resid 155 and name C)	6.00	0.24	0.25
	assign (segid 3A4 and resid 152 and name CA) (segid 3A4 and resid 155 and name CA)	5.35	0.25	0.24
	assign (segid 3A4 and resid 152 and name CA) (segid 3A4 and resid 155 and name CB)	4.75	0.38	0.38
5	assign (segid 3A4 and resid 152 and name CA) (segid 3A4 and resid 155 and name N)	4.70	0.15	0.16
	assign (segid 3A4 and resid 152 and name CA) (segid 3A4 and resid 155 and name O)	7.20	0.24	0.25
	assign (segid 3A4 and resid 152 and name CA) (segid 3A4 and resid 156 and name CA)	6.50	0.21	0.21
	assign (segid 3A4 and resid 152 and name CA) (segid 3A4 and resid 156 and name CB)	6.14	0.24	0.24
	assign (segid 3A4 and resid 152 and name CA) (segid 3A4 and resid 156 and name N)	5.48	0.22	0.22
10	assign (segid 3A4 and resid 152 and name CA) (segid 3A4 and resid 157 and name CA)	8.86	0.17	0.16
	assign (segid 3A4 and resid 152 and name CA) (segid 3A4 and resid 157 and name CB)	8.85	0.24	0.24
	assign (segid 3A4 and resid 152 and name CA) (segid 3A4 and resid 157 and name N)	7.59	0.16	0.16
	assign (segid 3A4 and resid 152 and name CA) (segid 3A4 and resid 158 and name CA)	10.17	0.25	0.25
	assign (segid 3A4 and resid 152 and name CA) (segid 3A4 and resid 158 and name CB)	9.78	0.25	0.26
15	assign (segid 3A4 and resid 152 and name CA) (segid 3A4 and resid 159 and name CA)	10.94	0.58	0.58
	assign (segid 3A4 and resid 152 and name CA) (segid 3A4 and resid 159 and name CB)	10.26	0.63	0.63
	assign (segid 3A4 and resid 152 and name CA) (segid 3A4 and resid 160 and name CA)	12.58	0.90	0.89
	assign (segid 3A4 and resid 152 and name CA) (segid 3A4 and resid 160 and name CB)	12.15	1.05	1.04
	assign (segid 3A4 and resid 152 and name CA) (segid 3A4 and resid 161 and name CA)	14.45	0.88	0.89
20	assign (segid 3A4 and resid 152 and name CA) (segid 3A4 and resid 161 and name CB)	14.19	0.91	0.90
	assign (segid 3A4 and resid 152 and name CA) (segid 3A4 and resid 161 and name N)	14.01	1.70	1.70
	assign (segid 3A4 and resid 152 and name CA) (segid 3A4 and resid 167 and name CB)	15.07	1.81	1.81
	assign (segid 3A4 and resid 152 and name CA) (segid 3A4 and resid 167 and name N)	15.23	1.55	1.55
	assign (segid 3A4 and resid 152 and name CA) (segid 3A4 and resid 168 and name CA)	13.20	1.25	1.26
25	assign (segid 3A4 and resid 152 and name CA) (segid 3A4 and resid 168 and name CB)	13.38	1.23	1.22
	assign (segid 3A4 and resid 152 and name CA) (segid 3A4 and resid 169 and name CA)	9.94	1.39	1.39
	assign (segid 3A4 and resid 152 and name CA) (segid 3A4 and resid 169 and name CB)	9.76	1.51	1.50
	assign (segid 3A4 and resid 152 and name CA) (segid 3A4 and resid 170 and name CA)	11.46	1.62	1.61
	assign (segid 3A4 and resid 152 and name CA) (segid 3A4 and resid 171 and name CB)	12.83	1.70	1.69
30	assign (segid 3A4 and resid 152 and name CA) (segid 3A4 and resid 172 and name CA)	12.55	1.26	1.27
	assign (segid 3A4 and resid 152 and name CA) (segid 3A4 and resid 172 and name CB)	13.50	1.27	1.28
	assign (segid 3A4 and resid 152 and name CA) (segid 3A4 and resid 173 and name CA)	9.46	1.03	1.03
	assign (segid 3A4 and resid 152 and name CA) (segid 3A4 and resid 173 and name CB)	8.61	1.04	1.05
	assign (segid 3A4 and resid 152 and name CA) (segid 3A4 and resid 174 and name CA)	8.41	1.19	1.19
35	assign (segid 3A4 and resid 152 and name CA) (segid 3A4 and resid 174 and name CB)	8.43	1.33	1.34
	assign (segid 3A4 and resid 152 and name CA) (segid 3A4 and resid 175 and name CA)	11.93	1.20	1.20
	assign (segid 3A4 and resid 152 and name CA) (segid 3A4 and resid 175 and name CB)	13.06	1.27	1.27
	assign (segid 3A4 and resid 152 and name CA) (segid 3A4 and resid 176 and name CA)	12.17	1.04	1.04
	assign (segid 3A4 and resid 152 and name CA) (segid 3A4 and resid 176 and name CB)	12.05	1.04	1.05
40	assign (segid 3A4 and resid 152 and name CA) (segid 3A4 and resid 177 and name CA)	9.87	1.16	1.16
	assign (segid 3A4 and resid 152 and name CA) (segid 3A4 and resid 177 and name CB)	8.51	1.23	1.23
	assign (segid 3A4 and resid 152 and name CA) (segid 3A4 and resid 178 and name CA)	11.81	1.09	1.08
	assign (segid 3A4 and resid 152 and name CA) (segid 3A4 and resid 178 and name CB)	11.95	1.16	1.16
	assign (segid 3A4 and resid 152 and name CA) (segid 3A4 and resid 179 and name CA)	14.88	1.02	1.03
45	assign (segid 3A4 and resid 152 and name CA) (segid 3A4 and resid 179 and name CB)	15.26	1.01	1.01
	assign (segid 3A4 and resid 152 and name CA) (segid 3A4 and resid 180 and name CA)	14.88	1.21	1.21
	assign (segid 3A4 and resid 152 and name CA) (segid 3A4 and resid 181 and name CA)	14.61	1.06	1.06
	assign (segid 3A4 and resid 152 and name CA) (segid 3A4 and resid 181 and name CB)	13.59	0.98	0.98
	assign (segid 3A4 and resid 152 and name CA) (segid 3A4 and resid 182 and name CA)	17.36	0.93	0.94
50	assign (segid 3A4 and resid 152 and name CA) (segid 3A4 and resid 182 and name CB)	17.44	0.96	0.97
	assign (segid 3A4 and resid 152 and name CA) (segid 3A4 and resid 183 and name CB)	18.67	0.60	0.59
	assign (segid 3A4 and resid 152 and name CA) (segid 3A4 and resid 184 and name CA)	18.32	0.82	0.82
	assign (segid 3A4 and resid 152 and name CA) (segid 3A4 and resid 184 and name CB)	17.17	0.81	0.81
	assign (segid 3A4 and resid 152 and name CA) (segid 3A4 and resid 185 and name CA)	16.27	1.77	1.78
55	assign (segid 3A4 and resid 152 and name CA) (segid 3A4 and resid 185 and name CB)	16.23	1.84	1.85
	assign (segid 3A4 and resid 152 and name CA) (segid 3A4 and resid 186 and name CA)	14.68	1.77	1.76
	assign (segid 3A4 and resid 152 and name CA) (segid 3A4 and resid 186 and name CB)	14.34	1.71	1.72
	assign (segid 3A4 and resid 152 and name CA) (segid 3A4 and resid 187 and name CA)	12.62	2.03	2.02
	assign (segid 3A4 and resid 152 and name CA) (segid 3A4 and resid 187 and name CB)	15.05	2.09	2.09
60	assign (segid 3A4 and resid 152 and name CA) (segid 3A4 and resid 188 and name CA)	15.08	1.64	1.65
	assign (segid 3A4 and resid 152 and name CA) (segid 3A4 and resid 188 and name CB)	15.54	1.57	1.56
	assign (segid 3A4 and resid 152 and name CA) (segid 3A4 and resid 189 and name CA)	11.53	1.55	1.54
	assign (segid 3A4 and resid 152 and name CA) (segid 3A4 and resid 189 and name CB)	10.44	1.59	1.59
	assign (segid 3A4 and resid 152 and name CA) (segid 3A4 and resid 190 and name CA)	11.82	1.95	1.96
65	assign (segid 3A4 and resid 152 and name CA) (segid 3A4 and resid 190 and name CB)	15.36	1.89	1.88
	assign (segid 3A4 and resid 152 and name CA) (segid 3A4 and resid 191 and name CA)	15.06	1.62	1.62
	assign (segid 3A4 and resid 152 and name CA) (segid 3A4 and resid 191 and name CB)	12.67	1.38	1.38
	assign (segid 3A4 and resid 152 and name CA) (segid 3A4 and resid 192 and name CA)	13.91	1.27	1.28
	assign (segid 3A4 and resid 152 and name CA) (segid 3A4 and resid 192 and name CB)	17.40	1.30	1.30
70	assign (segid 3A4 and resid 152 and name CA) (segid 3A4 and resid 193 and name CA)	17.80	0.84	0.83
	assign (segid 3A4 and resid 152 and name CA) (segid 3A4 and resid 193 and name CB)	17.39	0.83	0.83
	assign (segid 3A4 and resid 152 and name CA) (segid 3A4 and resid 194 and name CA)	16.28	0.76	0.75
	assign (segid 3A4 and resid 152 and name CA) (segid 3A4 and resid 194 and name CB)	15.00	0.83	0.83
75	assign (segid 3A4 and resid 152 and name CB) (segid 3A4 and resid 153 and name C)	5.45	0.07	0.07
	assign (segid 3A4 and resid 152 and name CB) (segid 3A4 and resid 153 and name CB)	4.45	0.07	0.07
	assign (segid 3A4 and resid 152 and name CB) (segid 3A4 and resid 153 and name N)	5.27	0.08	0.07
	assign (segid 3A4 and resid 152 and name CB) (segid 3A4 and resid 153 and name O)	3.11	0.08	0.09
	assign (segid 3A4 and resid 152 and name CB) (segid 3A4 and resid 153 and name C)	6.38	0.09	0.09
80	assign (segid 3A4 and resid 152 and name CB) (segid 3A4 and resid 154 and name C)	6.98	0.10	0.10
	assign (segid 3A4 and resid 152 and name CB) (segid 3A4 and resid 154 and name CA)	6.79	0.13	0.12
	assign (segid 3A4 and resid 152 and name CB) (segid 3A4 and resid 154 and name N)	5.57	0.13	0.12
	assign (segid 3A4 and resid 152 and name CB) (segid 3A4 and resid 155 and name C)	7.15	0.23	0.22

	assign (segid 3A4 and resid 152 and name CB)	(segid 3A4 and resid 155 and name CA)	6.67	0.24	0.24
	assign (segid 3A4 and resid 152 and name CB)	(segid 3A4 and resid 155 and name CB)	5.99	0.38	0.39
	assign (segid 3A4 and resid 152 and name CB)	(segid 3A4 and resid 155 and name N)	6.11	0.14	0.13
	assign (segid 3A4 and resid 152 and name CB)	(segid 3A4 and resid 156 and name CA)	7.27	0.18	0.18
	assign (segid 3A4 and resid 152 and name CB)	(segid 3A4 and resid 156 and name CB)	6.66	0.20	0.19
5	assign (segid 3A4 and resid 152 and name CB)	(segid 3A4 and resid 156 and name N)	6.47	0.19	0.18
	assign (segid 3A4 and resid 152 and name CB)	(segid 3A4 and resid 157 and name CA)	9.83	0.13	0.13
	assign (segid 3A4 and resid 152 and name CB)	(segid 3A4 and resid 157 and name CB)	9.85	0.24	0.24
	assign (segid 3A4 and resid 152 and name CB)	(segid 3A4 and resid 158 and name CA)	11.44	0.21	0.20
	assign (segid 3A4 and resid 152 and name CB)	(segid 3A4 and resid 158 and name CB)	11.14	0.22	0.22
10	assign (segid 3A4 and resid 152 and name CB)	(segid 3A4 and resid 159 and name CA)	11.97	0.51	0.51
	assign (segid 3A4 and resid 152 and name CB)	(segid 3A4 and resid 159 and name CB)	11.19	0.54	0.54
	assign (segid 3A4 and resid 152 and name CB)	(segid 3A4 and resid 160 and name CA)	13.39	0.89	0.90
	assign (segid 3A4 and resid 152 and name CB)	(segid 3A4 and resid 160 and name CB)	12.87	1.08	1.08
	assign (segid 3A4 and resid 152 and name CB)	(segid 3A4 and resid 161 and name CA)	15.48	0.95	0.94
15	assign (segid 3A4 and resid 152 and name CB)	(segid 3A4 and resid 161 and name CB)	15.25	1.00	1.01
	assign (segid 3A4 and resid 152 and name CB)	(segid 3A4 and resid 161 and name N)	14.69	1.36	1.36
	assign (segid 3A4 and resid 152 and name CB)	(segid 3A4 and resid 167 and name CB)	15.78	1.49	1.50
	assign (segid 3A4 and resid 152 and name CB)	(segid 3A4 and resid 188 and name CA)	15.65	1.15	1.14
	assign (segid 3A4 and resid 152 and name CB)	(segid 3A4 and resid 189 and name CA)	13.51	0.79	0.78
20	assign (segid 3A4 and resid 152 and name CB)	(segid 3A4 and resid 189 and name CB)	13.71	0.76	0.76
	assign (segid 3A4 and resid 152 and name CB)	(segid 3A4 and resid 190 and name CA)	10.40	1.00	1.00
	assign (segid 3A4 and resid 152 and name CB)	(segid 3A4 and resid 190 and name CB)	10.39	1.16	1.15
	assign (segid 3A4 and resid 152 and name CB)	(segid 3A4 and resid 191 and name CA)	11.73	1.34	1.34
	assign (segid 3A4 and resid 152 and name CB)	(segid 3A4 and resid 191 and name CB)	13.13	1.43	1.43
25	assign (segid 3A4 and resid 152 and name CB)	(segid 3A4 and resid 192 and name CA)	12.51	0.89	0.88
	assign (segid 3A4 and resid 152 and name CB)	(segid 3A4 and resid 192 and name CB)	13.46	0.86	0.86
	assign (segid 3A4 and resid 152 and name CB)	(segid 3A4 and resid 193 and name CA)	9.28	0.66	0.65
	assign (segid 3A4 and resid 152 and name CB)	(segid 3A4 and resid 193 and name CB)	8.55	0.65	0.64
	assign (segid 3A4 and resid 152 and name CB)	(segid 3A4 and resid 194 and name CA)	8.21	1.06	1.07
30	assign (segid 3A4 and resid 152 and name CB)	(segid 3A4 and resid 194 and name CB)	8.41	1.29	1.28
	assign (segid 3A4 and resid 152 and name CB)	(segid 3A4 and resid 195 and name CA)	11.57	1.08	1.08
	assign (segid 3A4 and resid 152 and name CB)	(segid 3A4 and resid 195 and name CB)	12.78	1.11	1.10
	assign (segid 3A4 and resid 152 and name CB)	(segid 3A4 and resid 196 and name CA)	11.54	0.95	0.94
	assign (segid 3A4 and resid 152 and name CB)	(segid 3A4 and resid 196 and name CB)	11.43	0.95	0.95
35	assign (segid 3A4 and resid 152 and name CB)	(segid 3A4 and resid 197 and name CA)	9.05	1.22	1.22
	assign (segid 3A4 and resid 152 and name CB)	(segid 3A4 and resid 197 and name CB)	7.73	1.27	1.27
	assign (segid 3A4 and resid 152 and name CB)	(segid 3A4 and resid 198 and name CA)	11.07	1.21	1.20
	assign (segid 3A4 and resid 152 and name CB)	(segid 3A4 and resid 198 and name CB)	11.33	1.29	1.29
	assign (segid 3A4 and resid 152 and name CB)	(segid 3A4 and resid 199 and name CA)	14.09	1.07	1.06
40	assign (segid 3A4 and resid 152 and name CB)	(segid 3A4 and resid 199 and name CB)	14.50	1.01	1.00
	assign (segid 3A4 and resid 152 and name CB)	(segid 3A4 and resid 200 and name CA)	13.91	1.30	1.29
	assign (segid 3A4 and resid 152 and name CB)	(segid 3A4 and resid 201 and name CA)	13.65	1.16	1.16
	assign (segid 3A4 and resid 152 and name CB)	(segid 3A4 and resid 201 and name CB)	12.67	1.09	1.09
	assign (segid 3A4 and resid 152 and name CB)	(segid 3A4 and resid 202 and name CA)	16.50	1.06	1.06
45	assign (segid 3A4 and resid 152 and name CB)	(segid 3A4 and resid 202 and name CB)	16.63	1.08	1.09
	assign (segid 3A4 and resid 152 and name CB)	(segid 3A4 and resid 203 and name CB)	18.23	1.07	1.07
	assign (segid 3A4 and resid 152 and name CB)	(segid 3A4 and resid 219 and name CB)	17.99	0.71	0.70
	assign (segid 3A4 and resid 152 and name CB)	(segid 3A4 and resid 221 and name CA)	17.65	1.01	1.01
	assign (segid 3A4 and resid 152 and name CB)	(segid 3A4 and resid 221 and name CB)	16.46	0.94	0.95
50	assign (segid 3A4 and resid 152 and name CB)	(segid 3A4 and resid 245 and name CA)	15.80	1.86	1.86
	assign (segid 3A4 and resid 152 and name CB)	(segid 3A4 and resid 245 and name CB)	15.74	1.86	1.87
	assign (segid 3A4 and resid 152 and name CB)	(segid 3A4 and resid 248 and name CA)	14.30	2.07	2.08
	assign (segid 3A4 and resid 152 and name CB)	(segid 3A4 and resid 248 and name CB)	13.88	1.99	1.98
	assign (segid 3A4 and resid 152 and name CB)	(segid 3A4 and resid 249 and name CA)	12.47	2.30	2.29
55	assign (segid 3A4 and resid 152 and name CB)	(segid 3A4 and resid 250 and name CA)	15.09	2.43	2.43
	assign (segid 3A4 and resid 152 and name CB)	(segid 3A4 and resid 251 and name CA)	15.02	2.13	2.13
	assign (segid 3A4 and resid 152 and name CB)	(segid 3A4 and resid 251 and name CB)	15.37	2.06	2.05
	assign (segid 3A4 and resid 152 and name CB)	(segid 3A4 and resid 252 and name CA)	11.51	2.09	2.08
	assign (segid 3A4 and resid 152 and name CB)	(segid 3A4 and resid 252 and name CB)	10.34	2.10	2.10
60	assign (segid 3A4 and resid 152 and name CB)	(segid 3A4 and resid 253 and name CA)	12.14	2.40	2.41
	assign (segid 3A4 and resid 152 and name CB)	(segid 3A4 and resid 253 and name CB)	15.69	2.35	2.35
	assign (segid 3A4 and resid 152 and name CB)	(segid 3A4 and resid 254 and name CA)	15.31	2.18	2.18
	assign (segid 3A4 and resid 152 and name CB)	(segid 3A4 and resid 255 and name CA)	13.09	1.95	1.94
	assign (segid 3A4 and resid 152 and name CB)	(segid 3A4 and resid 256 and name CA)	14.57	1.80	1.81
65	assign (segid 3A4 and resid 152 and name CB)	(segid 3A4 and resid 257 and name CA)	17.84	1.55	1.54
	assign (segid 3A4 and resid 152 and name CB)	(segid 3A4 and resid 259 and name CB)	16.95	1.33	1.33
	assign (segid 3A4 and resid 152 and name CB)	(segid 3A4 and resid 260 and name CA)	15.70	1.36	1.35
	assign (segid 3A4 and resid 152 and name CB)	(segid 3A4 and resid 260 and name CB)	2.45	0.02	0.03
	assign (segid 3A4 and resid 152 and name N)	(segid 3A4 and resid 152 and name C)	1.46	0.01	0.01
70	assign (segid 3A4 and resid 152 and name N)	(segid 3A4 and resid 152 and name CA)	2.44	0.03	0.03
	assign (segid 3A4 and resid 152 and name N)	(segid 3A4 and resid 152 and name CB)	3.45	0.07	0.06
	assign (segid 3A4 and resid 152 and name N)	(segid 3A4 and resid 153 and name C)	4.73	0.04	0.04
	assign (segid 3A4 and resid 152 and name N)	(segid 3A4 and resid 153 and name CA)	4.24	0.05	0.04
	assign (segid 3A4 and resid 152 and name N)	(segid 3A4 and resid 153 and name CB)	5.02	0.08	0.08
75	assign (segid 3A4 and resid 152 and name N)	(segid 3A4 and resid 153 and name N)	2.84	0.05	0.05
	assign (segid 3A4 and resid 152 and name N)	(segid 3A4 and resid 153 and name O)	5.84	0.08	0.08
	assign (segid 3A4 and resid 152 and name N)	(segid 3A4 and resid 154 and name C)	5.69	0.09	0.09
	assign (segid 3A4 and resid 152 and name N)	(segid 3A4 and resid 154 and name CA)	5.27	0.08	0.09
	assign (segid 3A4 and resid 152 and name N)	(segid 3A4 and resid 154 and name N)	4.27	0.08	0.08
80	assign (segid 3A4 and resid 152 and name N)	(segid 3A4 and resid 154 and name O)	6.90	0.10	0.10
	assign (segid 3A4 and resid 152 and name N)	(segid 3A4 and resid 155 and name C)	6.73	0.25	0.24
	assign (segid 3A4 and resid 152 and name N)	(segid 3A4 and resid 155 and name CA)	5.83	0.27	0.27

	assign (segid 3A4 and resid 152 and name N)	(segid 3A4 and resid 155 and name CB)	5.35	0.41	0.41
	assign (segid 3A4 and resid 152 and name N)	(segid 3A4 and resid 155 and name N)	4.96	0.17	0.17
	assign (segid 3A4 and resid 152 and name N)	(segid 3A4 and resid 156 and name CA)	7.50	0.20	0.20
	assign (segid 3A4 and resid 152 and name N)	(segid 3A4 and resid 156 and name CB)	7.24	0.22	0.23
	assign (segid 3A4 and resid 152 and name N)	(segid 3A4 and resid 156 and name N)	6.36	0.21	0.22
5	assign (segid 3A4 and resid 152 and name N)	(segid 3A4 and resid 152 and name CB)	3.36	0.07	0.06
	assign (segid 3A4 and resid 152 and name O)	(segid 3A4 and resid 153 and name C)	3.02	0.09	0.10
	assign (segid 3A4 and resid 152 and name O)	(segid 3A4 and resid 153 and name CA)	2.79	0.03	0.03
	assign (segid 3A4 and resid 152 and name O)	(segid 3A4 and resid 153 and name CB)	4.28	0.03	0.03
	assign (segid 3A4 and resid 152 and name O)	(segid 3A4 and resid 153 and name N)	2.26	0.02	0.02
10	assign (segid 3A4 and resid 152 and name O)	(segid 3A4 and resid 153 and name O)	3.58	0.12	0.13
	assign (segid 3A4 and resid 152 and name O)	(segid 3A4 and resid 154 and name C)	4.10	0.16	0.17
	assign (segid 3A4 and resid 152 and name O)	(segid 3A4 and resid 154 and name CA)	4.34	0.24	0.24
	assign (segid 3A4 and resid 152 and name O)	(segid 3A4 and resid 154 and name N)	3.37	0.24	0.24
	assign (segid 3A4 and resid 152 and name O)	(segid 3A4 and resid 154 and name O)	5.06	0.13	0.14
15	assign (segid 3A4 and resid 152 and name O)	(segid 3A4 and resid 155 and name C)	3.94	0.12	0.12
	assign (segid 3A4 and resid 152 and name O)	(segid 3A4 and resid 155 and name CA)	3.73	0.05	0.05
	assign (segid 3A4 and resid 152 and name O)	(segid 3A4 and resid 155 and name CB)	3.54	0.15	0.15
	assign (segid 3A4 and resid 152 and name O)	(segid 3A4 and resid 155 and name N)	3.23	0.13	0.13
	assign (segid 3A4 and resid 152 and name O)	(segid 3A4 and resid 155 and name O)	5.14	0.13	0.12
20	assign (segid 3A4 and resid 152 and name O)	(segid 3A4 and resid 156 and name C)	5.33	0.18	0.18
	assign (segid 3A4 and resid 152 and name O)	(segid 3A4 and resid 156 and name CA)	4.15	0.22	0.21
	assign (segid 3A4 and resid 152 and name O)	(segid 3A4 and resid 156 and name CB)	3.88	0.29	0.29
	assign (segid 3A4 and resid 152 and name O)	(segid 3A4 and resid 156 and name N)	3.19	0.16	0.17
	assign (segid 3A4 and resid 152 and name O)	(segid 3A4 and resid 156 and name O)	6.46	0.18	0.17
25	assign (segid 3A4 and resid 152 and name O)	(segid 3A4 and resid 157 and name C)	7.47	0.15	0.15
	assign (segid 3A4 and resid 152 and name O)	(segid 3A4 and resid 157 and name CA)	6.64	0.17	0.18
	assign (segid 3A4 and resid 152 and name O)	(segid 3A4 and resid 157 and name CB)	6.84	0.26	0.26
	assign (segid 3A4 and resid 152 and name O)	(segid 3A4 and resid 157 and name N)	5.31	0.16	0.17
	assign (segid 3A4 and resid 152 and name O)	(segid 3A4 and resid 157 and name O)	7.10	0.14	0.13
30	assign (segid 3A4 and resid 152 and name O)	(segid 3A4 and resid 158 and name N)	2.51	0.02	0.03
	assign (segid 3A4 and resid 153 and name C)	(segid 3A4 and resid 153 and name CB)	1.23	0.00	0.00
	assign (segid 3A4 and resid 153 and name C)	(segid 3A4 and resid 154 and name C)	2.99	0.08	0.08
	assign (segid 3A4 and resid 153 and name C)	(segid 3A4 and resid 154 and name CA)	2.44	0.02	0.02
	assign (segid 3A4 and resid 153 and name C)	(segid 3A4 and resid 154 and name N)	1.33	0.00	0.00
35	assign (segid 3A4 and resid 153 and name C)	(segid 3A4 and resid 154 and name O)	3.82	0.10	0.10
	assign (segid 3A4 and resid 153 and name C)	(segid 3A4 and resid 155 and name C)	4.48	0.11	0.12
	assign (segid 3A4 and resid 153 and name C)	(segid 3A4 and resid 155 and name CA)	4.40	0.13	0.13
	assign (segid 3A4 and resid 153 and name C)	(segid 3A4 and resid 155 and name CB)	5.17	0.16	0.16
	assign (segid 3A4 and resid 153 and name C)	(segid 3A4 and resid 155 and name N)	3.24	0.11	0.11
40	assign (segid 3A4 and resid 153 and name C)	(segid 3A4 and resid 155 and name O)	5.52	0.17	0.16
	assign (segid 3A4 and resid 153 and name C)	(segid 3A4 and resid 156 and name C)	4.91	0.06	0.06
	assign (segid 3A4 and resid 153 and name C)	(segid 3A4 and resid 156 and name CA)	4.53	0.09	0.08
	assign (segid 3A4 and resid 153 and name C)	(segid 3A4 and resid 156 and name CB)	4.29	0.16	0.16
	assign (segid 3A4 and resid 153 and name C)	(segid 3A4 and resid 156 and name N)	3.80	0.07	0.07
45	assign (segid 3A4 and resid 153 and name C)	(segid 3A4 and resid 156 and name O)	6.13	0.06	0.06
	assign (segid 3A4 and resid 153 and name C)	(segid 3A4 and resid 157 and name C)	6.06	0.08	0.09
	assign (segid 3A4 and resid 153 and name C)	(segid 3A4 and resid 157 and name CA)	5.04	0.10	0.11
	assign (segid 3A4 and resid 153 and name C)	(segid 3A4 and resid 157 and name CB)	4.64	0.21	0.21
	assign (segid 3A4 and resid 153 and name C)	(segid 3A4 and resid 157 and name N)	4.16	0.07	0.06
50	assign (segid 3A4 and resid 153 and name C)	(segid 3A4 and resid 157 and name O)	7.23	0.08	0.09
	assign (segid 3A4 and resid 153 and name C)	(segid 3A4 and resid 158 and name CA)	7.13	0.16	0.16
	assign (segid 3A4 and resid 153 and name C)	(segid 3A4 and resid 158 and name CB)	7.13	0.22	0.23
	assign (segid 3A4 and resid 153 and name C)	(segid 3A4 and resid 158 and name N)	5.88	0.12	0.12
	assign (segid 3A4 and resid 153 and name CA)	(segid 3A4 and resid 153 and name C)	1.52	0.01	0.00
55	assign (segid 3A4 and resid 153 and name CA)	(segid 3A4 and resid 153 and name CB)	1.53	0.00	0.01
	assign (segid 3A4 and resid 153 and name CA)	(segid 3A4 and resid 153 and name O)	2.40	0.01	0.01
	assign (segid 3A4 and resid 153 and name CA)	(segid 3A4 and resid 154 and name C)	4.38	0.06	0.05
	assign (segid 3A4 and resid 153 and name CA)	(segid 3A4 and resid 154 and name CA)	3.80	0.02	0.02
	assign (segid 3A4 and resid 153 and name CA)	(segid 3A4 and resid 154 and name N)	2.42	0.02	0.02
60	assign (segid 3A4 and resid 153 and name CA)	(segid 3A4 and resid 154 and name O)	5.28	0.10	0.09
	assign (segid 3A4 and resid 153 and name CA)	(segid 3A4 and resid 155 and name C)	5.41	0.13	0.13
	assign (segid 3A4 and resid 153 and name CA)	(segid 3A4 and resid 155 and name CB)	5.37	0.12	0.12
	assign (segid 3A4 and resid 153 and name CA)	(segid 3A4 and resid 155 and name N)	5.80	0.18	0.18
	assign (segid 3A4 and resid 153 and name CA)	(segid 3A4 and resid 155 and name O)	4.32	0.09	0.09
65	assign (segid 3A4 and resid 153 and name CA)	(segid 3A4 and resid 155 and name O)	6.51	0.16	0.16
	assign (segid 3A4 and resid 153 and name CA)	(segid 3A4 and resid 156 and name C)	5.70	0.06	0.07
	assign (segid 3A4 and resid 153 and name CA)	(segid 3A4 and resid 156 and name CA)	5.07	0.10	0.10
	assign (segid 3A4 and resid 153 and name CA)	(segid 3A4 and resid 156 and name CB)	4.41	0.17	0.16
	assign (segid 3A4 and resid 153 and name CA)	(segid 3A4 and resid 156 and name N)	4.50	0.10	0.10
70	assign (segid 3A4 and resid 153 and name CA)	(segid 3A4 and resid 156 and name O)	6.91	0.06	0.05
	assign (segid 3A4 and resid 153 and name CA)	(segid 3A4 and resid 157 and name C)	7.30	0.08	0.07
	assign (segid 3A4 and resid 153 and name CA)	(segid 3A4 and resid 157 and name CA)	6.14	0.10	0.10
	assign (segid 3A4 and resid 153 and name CA)	(segid 3A4 and resid 157 and name CB)	5.80	0.19	0.19
	assign (segid 3A4 and resid 153 and name CA)	(segid 3A4 and resid 157 and name N)	5.16	0.07	0.06
75	assign (segid 3A4 and resid 153 and name CA)	(segid 3A4 and resid 158 and name CA)	8.51	0.14	0.13
	assign (segid 3A4 and resid 153 and name CA)	(segid 3A4 and resid 158 and name CB)	8.54	0.18	0.19
	assign (segid 3A4 and resid 153 and name CA)	(segid 3A4 and resid 158 and name N)	7.22	0.11	0.11
	assign (segid 3A4 and resid 153 and name CA)	(segid 3A4 and resid 159 and name CA)	9.88	0.18	0.19
	assign (segid 3A4 and resid 153 and name CA)	(segid 3A4 and resid 159 and name CB)	9.55	0.15	0.15
80	assign (segid 3A4 and resid 153 and name CA)	(segid 3A4 and resid 160 and name CA)	10.70	0.37	0.37
	assign (segid 3A4 and resid 153 and name CA)	(segid 3A4 and resid 160 and name CB)	10.03	0.43	0.44
	assign (segid 3A4 and resid 153 and name CA)	(segid 3A4 and resid 161 and name CA)	12.26	0.72	0.72

	assign (segid 3A4 and resid 153 and name CA)	(segid 3A4 and resid 161 and name CB)	11.85	0.82	0.83
	assign (segid 3A4 and resid 153 and name CA)	(segid 3A4 and resid 187 and name CA)	13.48	1.40	1.40
	assign (segid 3A4 and resid 153 and name CA)	(segid 3A4 and resid 187 and name CB)	14.35	1.47	1.47
	assign (segid 3A4 and resid 153 and name CA)	(segid 3A4 and resid 188 and name CA)	15.00	1.14	1.14
5	assign (segid 3A4 and resid 153 and name CA)	(segid 3A4 and resid 189 and name CA)	13.52	1.23	1.22
	assign (segid 3A4 and resid 153 and name CA)	(segid 3A4 and resid 189 and name CB)	13.83	1.42	1.41
	assign (segid 3A4 and resid 153 and name CA)	(segid 3A4 and resid 190 and name CA)	9.97	1.19	1.20
	assign (segid 3A4 and resid 153 and name CA)	(segid 3A4 and resid 190 and name CB)	9.54	1.24	1.25
	assign (segid 3A4 and resid 153 and name CA)	(segid 3A4 and resid 191 and name CA)	11.05	0.73	0.73
10	assign (segid 3A4 and resid 153 and name CA)	(segid 3A4 and resid 191 and name CB)	12.27	0.66	0.66
	assign (segid 3A4 and resid 153 and name CA)	(segid 3A4 and resid 192 and name CA)	12.74	0.97	0.97
	assign (segid 3A4 and resid 153 and name CA)	(segid 3A4 and resid 192 and name CB)	13.82	0.94	0.94
	assign (segid 3A4 and resid 153 and name CA)	(segid 3A4 and resid 193 and name CA)	10.12	1.29	1.28
	assign (segid 3A4 and resid 153 and name CA)	(segid 3A4 and resid 193 and name CB)	9.39	1.33	1.34
15	assign (segid 3A4 and resid 153 and name CA)	(segid 3A4 and resid 194 and name CA)	8.31	1.18	1.18
	assign (segid 3A4 and resid 153 and name CA)	(segid 3A4 and resid 194 and name CB)	7.96	0.99	1.00
	assign (segid 3A4 and resid 153 and name CA)	(segid 3A4 and resid 195 and name CA)	11.81	1.09	1.10
	assign (segid 3A4 and resid 153 and name CA)	(segid 3A4 and resid 195 and name CB)	12.91	0.97	0.96
	assign (segid 3A4 and resid 153 and name CA)	(segid 3A4 and resid 196 and name CA)	12.79	1.50	1.49
20	assign (segid 3A4 and resid 153 and name CA)	(segid 3A4 and resid 196 and name CB)	12.91	1.54	1.54
	assign (segid 3A4 and resid 153 and name CA)	(segid 3A4 and resid 197 and name CA)	10.47	1.86	1.87
	assign (segid 3A4 and resid 153 and name CA)	(segid 3A4 and resid 197 and name CB)	9.03	1.97	1.97
	assign (segid 3A4 and resid 153 and name CA)	(segid 3A4 and resid 198 and name CA)	11.69	1.56	1.55
	assign (segid 3A4 and resid 153 and name CA)	(segid 3A4 and resid 198 and name CB)	11.55	1.34	1.35
25	assign (segid 3A4 and resid 153 and name CA)	(segid 3A4 and resid 199 and name CA)	15.09	1.47	1.46
	assign (segid 3A4 and resid 153 and name CA)	(segid 3A4 and resid 199 and name CB)	15.56	1.37	1.37
	assign (segid 3A4 and resid 153 and name CA)	(segid 3A4 and resid 201 and name CA)	14.85	2.07	2.06
	assign (segid 3A4 and resid 153 and name CA)	(segid 3A4 and resid 201 and name CB)	13.64	2.10	2.09
	assign (segid 3A4 and resid 153 and name CA)	(segid 3A4 and resid 245 and name CA)	15.47	0.87	0.87
30	assign (segid 3A4 and resid 153 and name CA)	(segid 3A4 and resid 245 and name CB)	15.62	0.86	0.86
	assign (segid 3A4 and resid 153 and name CA)	(segid 3A4 and resid 246 and name CA)	15.62	0.67	0.66
	assign (segid 3A4 and resid 153 and name CA)	(segid 3A4 and resid 246 and name CB)	16.86	0.70	0.70
	assign (segid 3A4 and resid 153 and name CA)	(segid 3A4 and resid 247 and name CA)	16.12	0.75	0.76
	assign (segid 3A4 and resid 153 and name CA)	(segid 3A4 and resid 247 and name CB)	17.27	0.83	0.83
35	assign (segid 3A4 and resid 153 and name CA)	(segid 3A4 and resid 248 and name CA)	13.25	1.01	1.01
	assign (segid 3A4 and resid 153 and name CA)	(segid 3A4 and resid 248 and name CB)	13.16	1.20	1.19
	assign (segid 3A4 and resid 153 and name CA)	(segid 3A4 and resid 249 and name CA)	11.07	0.73	0.73
	assign (segid 3A4 and resid 153 and name CA)	(segid 3A4 and resid 250 and name CA)	13.03	0.80	0.81
	assign (segid 3A4 and resid 153 and name CA)	(segid 3A4 and resid 250 and name CB)	14.49	0.81	0.81
40	assign (segid 3A4 and resid 153 and name CA)	(segid 3A4 and resid 251 and name CA)	12.95	0.73	0.73
	assign (segid 3A4 and resid 153 and name CA)	(segid 3A4 and resid 251 and name CB)	13.53	0.78	0.79
	assign (segid 3A4 and resid 153 and name CA)	(segid 3A4 and resid 252 and name CA)	9.33	0.78	0.79
	assign (segid 3A4 and resid 153 and name CA)	(segid 3A4 and resid 252 and name CB)	8.41	0.82	0.83
	assign (segid 3A4 and resid 153 and name CA)	(segid 3A4 and resid 253 and name CA)	9.39	0.99	0.98
45	assign (segid 3A4 and resid 153 and name CA)	(segid 3A4 and resid 254 and name CA)	12.77	1.05	1.05
	assign (segid 3A4 and resid 153 and name CA)	(segid 3A4 and resid 255 and name CA)	12.56	1.25	1.24
	assign (segid 3A4 and resid 153 and name CA)	(segid 3A4 and resid 256 and name CA)	10.14	1.18	1.18
	assign (segid 3A4 and resid 153 and name CA)	(segid 3A4 and resid 257 and name CA)	11.21	1.17	1.17
	assign (segid 3A4 and resid 153 and name CA)	(segid 3A4 and resid 258 and name CA)	14.70	1.07	1.07
50	assign (segid 3A4 and resid 153 and name CA)	(segid 3A4 and resid 258 and name CB)	15.32	1.08	1.08
	assign (segid 3A4 and resid 153 and name CA)	(segid 3A4 and resid 259 and name CA)	15.31	0.66	0.67
	assign (segid 3A4 and resid 153 and name CA)	(segid 3A4 and resid 259 and name CB)	14.97	0.63	0.63
	assign (segid 3A4 and resid 153 and name CA)	(segid 3A4 and resid 260 and name CA)	13.95	0.91	0.91
	assign (segid 3A4 and resid 153 and name CA)	(segid 3A4 and resid 260 and name CB)	12.68	1.02	1.02
55	assign (segid 3A4 and resid 153 and name CA)	(segid 3A4 and resid 261 and name CA)	16.09	1.29	1.30
	assign (segid 3A4 and resid 153 and name CA)	(segid 3A4 and resid 263 and name CA)	18.97	0.91	0.92
	assign (segid 3A4 and resid 153 and name CA)	(segid 3A4 and resid 263 and name CB)	18.04	0.89	0.90
	assign (segid 3A4 and resid 153 and name CB)	(segid 3A4 and resid 154 and name C)	5.43	0.07	0.08
	assign (segid 3A4 and resid 153 and name CB)	(segid 3A4 and resid 154 and name CA)	4.54	0.06	0.06
60	assign (segid 3A4 and resid 153 and name CB)	(segid 3A4 and resid 154 and name N)	3.23	0.09	0.08
	assign (segid 3A4 and resid 153 and name CB)	(segid 3A4 and resid 154 and name O)	6.27	0.12	0.11
	assign (segid 3A4 and resid 153 and name CB)	(segid 3A4 and resid 155 and name C)	6.80	0.15	0.15
	assign (segid 3A4 and resid 153 and name CB)	(segid 3A4 and resid 155 and name CA)	6.76	0.12	0.13
	assign (segid 3A4 and resid 153 and name CB)	(segid 3A4 and resid 155 and name CB)	7.28	0.20	0.19
65	assign (segid 3A4 and resid 153 and name CB)	(segid 3A4 and resid 155 and name N)	5.61	0.10	0.10
	assign (segid 3A4 and resid 153 and name CB)	(segid 3A4 and resid 156 and name C)	6.75	0.16	0.16
	assign (segid 3A4 and resid 153 and name CB)	(segid 3A4 and resid 156 and name CA)	6.31	0.17	0.18
	assign (segid 3A4 and resid 153 and name CB)	(segid 3A4 and resid 156 and name CB)	5.52	0.24	0.24
	assign (segid 3A4 and resid 153 and name CB)	(segid 3A4 and resid 156 and name N)	5.89	0.14	0.14
70	assign (segid 3A4 and resid 153 and name CB)	(segid 3A4 and resid 157 and name CA)	6.80	0.18	0.18
	assign (segid 3A4 and resid 153 and name CB)	(segid 3A4 and resid 157 and name CB)	6.19	0.23	0.23
	assign (segid 3A4 and resid 153 and name CB)	(segid 3A4 and resid 157 and name N)	6.04	0.16	0.17
	assign (segid 3A4 and resid 153 and name CB)	(segid 3A4 and resid 158 and name CA)	9.43	0.17	0.17
	assign (segid 3A4 and resid 153 and name CB)	(segid 3A4 and resid 158 and name CB)	9.54	0.26	0.25
75	assign (segid 3A4 and resid 153 and name CB)	(segid 3A4 and resid 159 and name CA)	11.04	0.16	0.16
	assign (segid 3A4 and resid 153 and name CB)	(segid 3A4 and resid 159 and name CB)	10.79	0.14	0.13
	assign (segid 3A4 and resid 153 and name CB)	(segid 3A4 and resid 160 and name CA)	11.56	0.35	0.35
	assign (segid 3A4 and resid 153 and name CB)	(segid 3A4 and resid 160 and name CB)	10.78	0.43	0.43
	assign (segid 3A4 and resid 153 and name CB)	(segid 3A4 and resid 161 and name CA)	12.97	0.68	0.67
80	assign (segid 3A4 and resid 153 and name CB)	(segid 3A4 and resid 161 and name CB)	12.48	0.77	0.77
	assign (segid 3A4 and resid 153 and name CB)	(segid 3A4 and resid 187 and name CA)	14.53	1.50	1.50
	assign (segid 3A4 and resid 153 and name CB)	(segid 3A4 and resid 187 and name CB)	15.38	1.55	1.55
	assign (segid 3A4 and resid 153 and name CB)	(segid 3A4 and resid 188 and name CA)	15.95	1.33	1.32

	assign (segid 3A4 and resid 153 and name CB)	(segid 3A4 and resid 189 and name CA)	14.49	1.41	1.41
	assign (segid 3A4 and resid 153 and name CB)	(segid 3A4 and resid 189 and name CB)	14.84	1.57	1.56
	assign (segid 3A4 and resid 153 and name CB)	(segid 3A4 and resid 190 and name CA)	10.99	1.38	1.38
	assign (segid 3A4 and resid 153 and name CB)	(segid 3A4 and resid 190 and name CB)	10.62	1.40	1.40
5	assign (segid 3A4 and resid 153 and name CB)	(segid 3A4 and resid 191 and name CA)	11.85	1.08	1.08
	assign (segid 3A4 and resid 153 and name CB)	(segid 3A4 and resid 191 and name CB)	13.06	0.99	0.99
	assign (segid 3A4 and resid 153 and name CB)	(segid 3A4 and resid 192 and name CA)	13.42	1.34	1.35
	assign (segid 3A4 and resid 153 and name CB)	(segid 3A4 and resid 192 and name CB)	14.55	1.26	1.26
	assign (segid 3A4 and resid 153 and name CB)	(segid 3A4 and resid 193 and name CA)	10.81	1.55	1.55
10	assign (segid 3A4 and resid 153 and name CB)	(segid 3A4 and resid 193 and name CB)	10.20	1.52	1.51
	assign (segid 3A4 and resid 153 and name CB)	(segid 3A4 and resid 194 and name CA)	8.77	1.68	1.67
	assign (segid 3A4 and resid 153 and name CB)	(segid 3A4 and resid 194 and name CB)	8.45	1.55	1.55
	assign (segid 3A4 and resid 153 and name CB)	(segid 3A4 and resid 195 and name CA)	12.12	1.67	1.68
	assign (segid 3A4 and resid 153 and name CB)	(segid 3A4 and resid 195 and name CB)	13.28	1.55	1.55
15	assign (segid 3A4 and resid 153 and name CB)	(segid 3A4 and resid 196 and name CA)	13.07	1.93	1.93
	assign (segid 3A4 and resid 153 and name CB)	(segid 3A4 and resid 196 and name CB)	13.29	1.90	1.90
	assign (segid 3A4 and resid 153 and name CB)	(segid 3A4 and resid 197 and name CA)	10.51	2.29	2.29
	assign (segid 3A4 and resid 153 and name CB)	(segid 3A4 and resid 197 and name CB)	9.07	2.36	2.36
	assign (segid 3A4 and resid 153 and name CB)	(segid 3A4 and resid 198 and name CA)	11.50	2.15	2.16
20	assign (segid 3A4 and resid 153 and name CB)	(segid 3A4 and resid 198 and name CB)	11.40	1.98	1.99
	assign (segid 3A4 and resid 153 and name CB)	(segid 3A4 and resid 199 and name CA)	15.01	2.08	2.07
	assign (segid 3A4 and resid 153 and name CB)	(segid 3A4 and resid 199 and name CB)	15.59	1.96	1.96
	assign (segid 3A4 and resid 153 and name CB)	(segid 3A4 and resid 201 and name CA)	13.14	2.68	2.68
	assign (segid 3A4 and resid 153 and name CB)	(segid 3A4 and resid 201 and name CB)	15.38	1.37	1.37
25	assign (segid 3A4 and resid 153 and name CB)	(segid 3A4 and resid 245 and name CA)	15.61	1.32	1.32
	assign (segid 3A4 and resid 153 and name CB)	(segid 3A4 and resid 246 and name CA)	15.66	1.03	1.02
	assign (segid 3A4 and resid 153 and name CB)	(segid 3A4 and resid 246 and name CB)	16.94	0.99	0.99
	assign (segid 3A4 and resid 153 and name CB)	(segid 3A4 and resid 247 and name CA)	15.94	1.14	1.14
	assign (segid 3A4 and resid 153 and name CB)	(segid 3A4 and resid 247 and name CB)	17.02	1.23	1.23
30	assign (segid 3A4 and resid 153 and name CB)	(segid 3A4 and resid 248 and name CA)	12.93	1.42	1.43
	assign (segid 3A4 and resid 153 and name CB)	(segid 3A4 and resid 248 and name CB)	12.81	1.62	1.62
	assign (segid 3A4 and resid 153 and name CB)	(segid 3A4 and resid 249 and name CA)	11.03	1.10	1.10
	assign (segid 3A4 and resid 153 and name CB)	(segid 3A4 and resid 250 and name CA)	12.98	1.05	1.04
	assign (segid 3A4 and resid 153 and name CB)	(segid 3A4 and resid 250 and name CB)	14.43	1.04	1.04
35	assign (segid 3A4 and resid 153 and name CB)	(segid 3A4 and resid 251 and name CA)	12.59	1.07	1.07
	assign (segid 3A4 and resid 153 and name CB)	(segid 3A4 and resid 251 and name CB)	13.08	1.16	1.17
	assign (segid 3A4 and resid 153 and name CB)	(segid 3A4 and resid 252 and name CA)	8.97	1.11	1.11
	assign (segid 3A4 and resid 153 and name CB)	(segid 3A4 and resid 252 and name CB)	8.08	1.18	1.19
	assign (segid 3A4 and resid 153 and name CB)	(segid 3A4 and resid 253 and name CA)	9.42	1.07	1.07
40	assign (segid 3A4 and resid 153 and name CB)	(segid 3A4 and resid 254 and name CA)	12.65	1.08	1.07
	assign (segid 3A4 and resid 153 and name CB)	(segid 3A4 and resid 255 and name CA)	12.20	1.44	1.44
	assign (segid 3A4 and resid 153 and name CB)	(segid 3A4 and resid 256 and name CA)	9.85	1.23	1.24
	assign (segid 3A4 and resid 153 and name CB)	(segid 3A4 and resid 257 and name CA)	11.16	1.28	1.28
	assign (segid 3A4 and resid 153 and name CB)	(segid 3A4 and resid 258 and name CA)	14.56	1.13	1.13
45	assign (segid 3A4 and resid 153 and name CB)	(segid 3A4 and resid 258 and name CB)	15.17	1.10	1.10
	assign (segid 3A4 and resid 153 and name CB)	(segid 3A4 and resid 259 and name CA)	14.96	0.77	0.78
	assign (segid 3A4 and resid 153 and name CB)	(segid 3A4 and resid 259 and name CB)	14.55	0.71	0.72
	assign (segid 3A4 and resid 153 and name CB)	(segid 3A4 and resid 260 and name CA)	13.67	1.13	1.13
	assign (segid 3A4 and resid 153 and name CB)	(segid 3A4 and resid 260 and name CB)	12.44	1.27	1.27
50	assign (segid 3A4 and resid 153 and name CB)	(segid 3A4 and resid 261 and name CA)	15.97	1.54	1.54
	assign (segid 3A4 and resid 153 and name CB)	(segid 3A4 and resid 263 and name CA)	17.64	1.14	1.13
	assign (segid 3A4 and resid 153 and name CB)	(segid 3A4 and resid 397 and name CA)	18.68	0.73	0.73
	assign (segid 3A4 and resid 153 and name CB)	(segid 3A4 and resid 397 and name CB)	18.71	0.67	0.68
	assign (segid 3A4 and resid 153 and name CB)	(segid 3A4 and resid 400 and name CB)	17.68	1.10	1.09
55	assign (segid 3A4 and resid 153 and name N)	(segid 3A4 and resid 153 and name C)	2.47	0.02	0.02
	assign (segid 3A4 and resid 153 and name N)	(segid 3A4 and resid 153 and name CA)	1.46	0.00	0.00
	assign (segid 3A4 and resid 153 and name N)	(segid 3A4 and resid 153 and name CB)	2.46	0.02	0.02
	assign (segid 3A4 and resid 153 and name N)	(segid 3A4 and resid 153 and name O)	3.54	0.04	0.03
60	assign (segid 3A4 and resid 153 and name N)	(segid 3A4 and resid 154 and name C)	4.71	0.07	0.07
	assign (segid 3A4 and resid 153 and name N)	(segid 3A4 and resid 154 and name CA)	4.19	0.05	0.05
	assign (segid 3A4 and resid 153 and name N)	(segid 3A4 and resid 154 and name CB)	2.78	0.05	0.06
	assign (segid 3A4 and resid 153 and name N)	(segid 3A4 and resid 154 and name O)	5.80	0.08	0.07
	assign (segid 3A4 and resid 153 and name N)	(segid 3A4 and resid 155 and name C)	5.67	0.15	0.15
	assign (segid 3A4 and resid 153 and name N)	(segid 3A4 and resid 155 and name CA)	5.35	0.16	0.16
65	assign (segid 3A4 and resid 153 and name N)	(segid 3A4 and resid 155 and name CB)	5.42	0.27	0.27
	assign (segid 3A4 and resid 153 and name N)	(segid 3A4 and resid 155 and name O)	4.33	0.12	0.11
	assign (segid 3A4 and resid 153 and name N)	(segid 3A4 and resid 156 and name C)	6.87	0.16	0.15
	assign (segid 3A4 and resid 153 and name N)	(segid 3A4 and resid 156 and name CA)	6.57	0.06	0.06
	assign (segid 3A4 and resid 153 and name N)	(segid 3A4 and resid 156 and name CB)	5.69	0.10	0.09
70	assign (segid 3A4 and resid 153 and name N)	(segid 3A4 and resid 156 and name O)	5.11	0.15	0.14
	assign (segid 3A4 and resid 153 and name N)	(segid 3A4 and resid 157 and name C)	4.89	0.12	0.12
	assign (segid 3A4 and resid 153 and name N)	(segid 3A4 and resid 157 and name CA)	7.78	0.06	0.06
	assign (segid 3A4 and resid 153 and name N)	(segid 3A4 and resid 157 and name CB)	7.28	0.10	0.10
	assign (segid 3A4 and resid 153 and name N)	(segid 3A4 and resid 157 and name O)	7.04	0.21	0.20
75	assign (segid 3A4 and resid 153 and name N)	(segid 3A4 and resid 157 and name N)	6.18	0.07	0.06
	assign (segid 3A4 and resid 153 and name O)	(segid 3A4 and resid 153 and name CB)	3.26	0.07	0.07
	assign (segid 3A4 and resid 153 and name O)	(segid 3A4 and resid 154 and name C)	2.94	0.13	0.13
	assign (segid 3A4 and resid 153 and name O)	(segid 3A4 and resid 154 and name CA)	2.78	0.03	0.02
	assign (segid 3A4 and resid 153 and name O)	(segid 3A4 and resid 154 and name N)	2.25	0.01	0.01
80	assign (segid 3A4 and resid 153 and name O)	(segid 3A4 and resid 154 and name O)	3.40	0.16	0.16
	assign (segid 3A4 and resid 153 and name O)	(segid 3A4 and resid 155 and name C)	4.02	0.21	0.22
	assign (segid 3A4 and resid 153 and name O)	(segid 3A4 and resid 155 and name CA)	4.31	0.22	0.22
	assign (segid 3A4 and resid 153 and name O)	(segid 3A4 and resid 155 and name CB)	5.30	0.24	0.25

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	assign (segid 3A4 and resid 154 and name CA)	(segid 3A4 and resid 195 and name CA)	13.98	0.54	0.53
	assign (segid 3A4 and resid 154 and name CA)	(segid 3A4 and resid 195 and name CB)	14.86	0.56	0.57
	assign (segid 3A4 and resid 154 and name CA)	(segid 3A4 and resid 196 and name CA)	15.17	0.80	0.81
	assign (segid 3A4 and resid 154 and name CA)	(segid 3A4 and resid 196 and name CB)	15.17	0.93	0.93
5	assign (segid 3A4 and resid 154 and name CA)	(segid 3A4 and resid 197 and name CA)	13.25	1.11	1.11
	assign (segid 3A4 and resid 154 and name CA)	(segid 3A4 and resid 197 and name CB)	11.83	1.25	1.26
	assign (segid 3A4 and resid 154 and name CA)	(segid 3A4 and resid 198 and name CA)	14.49	0.95	0.96
	assign (segid 3A4 and resid 154 and name CA)	(segid 3A4 and resid 198 and name CB)	14.24	0.81	0.81
	assign (segid 3A4 and resid 154 and name CA)	(segid 3A4 and resid 199 and name CA)	17.81	0.69	0.70
	assign (segid 3A4 and resid 154 and name CA)	(segid 3A4 and resid 199 and name CB)	18.19	0.52	0.52
10	assign (segid 3A4 and resid 154 and name CA)	(segid 3A4 and resid 245 and name CA)	17.83	0.55	0.56
	assign (segid 3A4 and resid 154 and name CA)	(segid 3A4 and resid 245 and name CB)	17.97	0.57	0.56
	assign (segid 3A4 and resid 154 and name CA)	(segid 3A4 and resid 246 and name CA)	17.54	0.46	0.45
	assign (segid 3A4 and resid 154 and name CA)	(segid 3A4 and resid 246 and name CB)	18.67	0.57	0.56
	assign (segid 3A4 and resid 154 and name CA)	(segid 3A4 and resid 247 and name CA)	18.07	0.58	0.57
15	assign (segid 3A4 and resid 154 and name CA)	(segid 3A4 and resid 248 and name CA)	15.49	0.92	0.92
	assign (segid 3A4 and resid 154 and name CA)	(segid 3A4 and resid 248 and name CB)	15.56	1.03	1.04
	assign (segid 3A4 and resid 154 and name CA)	(segid 3A4 and resid 249 and name CA)	13.01	0.56	0.57
	assign (segid 3A4 and resid 154 and name CA)	(segid 3A4 and resid 250 and name CA)	14.45	0.71	0.71
	assign (segid 3A4 and resid 154 and name CA)	(segid 3A4 and resid 250 and name CB)	15.88	0.70	0.70
20	assign (segid 3A4 and resid 154 and name CA)	(segid 3A4 and resid 251 and name CA)	14.50	1.11	1.10
	assign (segid 3A4 and resid 154 and name CA)	(segid 3A4 and resid 251 and name CB)	15.27	1.17	1.17
	assign (segid 3A4 and resid 154 and name CA)	(segid 3A4 and resid 252 and name CA)	10.93	1.23	1.24
	assign (segid 3A4 and resid 154 and name CA)	(segid 3A4 and resid 252 and name CB)	10.29	1.13	1.13
	assign (segid 3A4 and resid 154 and name CA)	(segid 3A4 and resid 253 and name CA)	10.20	0.97	0.96
25	assign (segid 3A4 and resid 154 and name CA)	(segid 3A4 and resid 254 and name CA)	13.33	1.12	1.11
	assign (segid 3A4 and resid 154 and name CA)	(segid 3A4 and resid 255 and name CA)	13.18	1.67	1.67
	assign (segid 3A4 and resid 154 and name CA)	(segid 3A4 and resid 256 and name CA)	10.25	1.94	1.93
	assign (segid 3A4 and resid 154 and name CA)	(segid 3A4 and resid 257 and name CA)	10.65	1.52	1.52
	assign (segid 3A4 and resid 154 and name CA)	(segid 3A4 and resid 258 and name CA)	14.20	1.41	1.41
30	assign (segid 3A4 and resid 154 and name CA)	(segid 3A4 and resid 258 and name CB)	15.02	1.31	1.31
	assign (segid 3A4 and resid 154 and name CA)	(segid 3A4 and resid 259 and name CA)	14.88	1.71	1.70
	assign (segid 3A4 and resid 154 and name CA)	(segid 3A4 and resid 259 and name CB)	14.73	1.83	1.84
	assign (segid 3A4 and resid 154 and name CA)	(segid 3A4 and resid 260 and name CA)	13.04	1.91	1.91
	assign (segid 3A4 and resid 154 and name CA)	(segid 3A4 and resid 260 and name CB)	11.70	1.96	1.96
35	assign (segid 3A4 and resid 154 and name CA)	(segid 3A4 and resid 261 and name CA)	14.89	1.44	1.43
	assign (segid 3A4 and resid 154 and name CA)	(segid 3A4 and resid 434 and name CA)	16.47	1.54	1.55
	assign (segid 3A4 and resid 154 and name CA)	(segid 3A4 and resid 435 and name CA)	17.20	1.59	1.59
	assign (segid 3A4 and resid 154 and name CA)	(segid 3A4 and resid 437 and name CA)	16.87	1.54	1.54
40	assign (segid 3A4 and resid 154 and name CA)	(segid 3A4 and resid 154 and name C)	2.43	0.02	0.02
	assign (segid 3A4 and resid 154 and name N)	(segid 3A4 and resid 154 and name CA)	1.46	0.01	0.01
	assign (segid 3A4 and resid 154 and name N)	(segid 3A4 and resid 154 and name O)	3.47	0.03	0.04
	assign (segid 3A4 and resid 154 and name N)	(segid 3A4 and resid 155 and name C)	4.68	0.05	0.05
	assign (segid 3A4 and resid 154 and name N)	(segid 3A4 and resid 155 and name CA)	4.18	0.05	0.04
	assign (segid 3A4 and resid 154 and name N)	(segid 3A4 and resid 155 and name CB)	4.94	0.08	0.07
45	assign (segid 3A4 and resid 154 and name N)	(segid 3A4 and resid 155 and name N)	2.78	0.04	0.04
	assign (segid 3A4 and resid 154 and name N)	(segid 3A4 and resid 155 and name O)	5.72	0.09	0.09
	assign (segid 3A4 and resid 154 and name N)	(segid 3A4 and resid 156 and name C)	5.70	0.12	0.11
	assign (segid 3A4 and resid 154 and name N)	(segid 3A4 and resid 156 and name CA)	5.34	0.14	0.14
	assign (segid 3A4 and resid 154 and name N)	(segid 3A4 and resid 156 and name CB)	5.36	0.19	0.19
50	assign (segid 3A4 and resid 154 and name N)	(segid 3A4 and resid 156 and name N)	4.33	0.13	0.14
	assign (segid 3A4 and resid 154 and name N)	(segid 3A4 and resid 156 and name O)	6.91	0.11	0.11
	assign (segid 3A4 and resid 154 and name N)	(segid 3A4 and resid 157 and name C)	6.47	0.14	0.15
	assign (segid 3A4 and resid 154 and name N)	(segid 3A4 and resid 157 and name CA)	5.68	0.15	0.16
	assign (segid 3A4 and resid 154 and name N)	(segid 3A4 and resid 157 and name CB)	5.17	0.29	0.29
55	assign (segid 3A4 and resid 154 and name N)	(segid 3A4 and resid 157 and name N)	4.90	0.12	0.12
	assign (segid 3A4 and resid 154 and name N)	(segid 3A4 and resid 157 and name O)	7.67	0.15	0.15
	assign (segid 3A4 and resid 154 and name N)	(segid 3A4 and resid 158 and name CA)	7.14	0.23	0.23
	assign (segid 3A4 and resid 154 and name N)	(segid 3A4 and resid 158 and name CB)	6.90	0.31	0.31
	assign (segid 3A4 and resid 154 and name N)	(segid 3A4 and resid 158 and name N)	6.05	0.17	0.18
60	assign (segid 3A4 and resid 154 and name N)	(segid 3A4 and resid 155 and name C)	3.01	0.06	0.06
	assign (segid 3A4 and resid 154 and name O)	(segid 3A4 and resid 155 and name CA)	2.76	0.01	0.02
	assign (segid 3A4 and resid 154 and name O)	(segid 3A4 and resid 155 and name CB)	4.25	0.01	0.02
	assign (segid 3A4 and resid 154 and name O)	(segid 3A4 and resid 155 and name N)	2.24	0.01	0.01
	assign (segid 3A4 and resid 154 and name O)	(segid 3A4 and resid 155 and name O)	3.43	0.13	0.13
65	assign (segid 3A4 and resid 154 and name O)	(segid 3A4 and resid 156 and name C)	4.29	0.15	0.15
	assign (segid 3A4 and resid 154 and name O)	(segid 3A4 and resid 156 and name CA)	4.52	0.16	0.16
	assign (segid 3A4 and resid 154 and name O)	(segid 3A4 and resid 156 and name CB)	5.46	0.16	0.16
	assign (segid 3A4 and resid 154 and name O)	(segid 3A4 and resid 156 and name N)	3.56	0.17	0.16
	assign (segid 3A4 and resid 154 and name O)	(segid 3A4 and resid 156 and name O)	5.18	0.16	0.15
70	assign (segid 3A4 and resid 154 and name O)	(segid 3A4 and resid 157 and name C)	3.97	0.13	0.12
	assign (segid 3A4 and resid 154 and name O)	(segid 3A4 and resid 157 and name CA)	3.98	0.14	0.14
	assign (segid 3A4 and resid 154 and name O)	(segid 3A4 and resid 157 and name CB)	3.94	0.33	0.32
	assign (segid 3A4 and resid 154 and name O)	(segid 3A4 and resid 157 and name N)	3.53	0.11	0.12
	assign (segid 3A4 and resid 154 and name O)	(segid 3A4 and resid 157 and name O)	5.13	0.14	0.13
75	assign (segid 3A4 and resid 154 and name O)	(segid 3A4 and resid 158 and name C)	4.95	0.40	0.40
	assign (segid 3A4 and resid 154 and name O)	(segid 3A4 and resid 158 and name CA)	7.84	0.21	0.22
	assign (segid 3A4 and resid 154 and name O)	(segid 3A4 and resid 158 and name CB)	3.51	0.24	0.23
	assign (segid 3A4 and resid 154 and name O)	(segid 3A4 and resid 158 and name N)	3.07	0.16	0.16
	assign (segid 3A4 and resid 154 and name O)	(segid 3A4 and resid 158 and name O)	6.07	0.36	0.36
80	assign (segid 3A4 and resid 154 and name O)	(segid 3A4 and resid 159 and name C)	7.19	0.57	0.57
	assign (segid 3A4 and resid 154 and name O)	(segid 3A4 and resid 159 and name CA)	6.29	0.57	0.57
	assign (segid 3A4 and resid 154 and name O)	(segid 3A4 and resid 159 and name CB)	6.56	0.61	0.60

	assign (segid 3A4 and resid 154 and name O)	(segid 3A4 and resid 159 and name N)	4.94	0.53	0.53
	assign (segid 3A4 and resid 154 and name O)	(segid 3A4 and resid 160 and name N)	6.93	0.50	0.51
	assign (segid 3A4 and resid 155 and name C)	(segid 3A4 and resid 155 and name CB)	2.52	0.01	0.01
	assign (segid 3A4 and resid 155 and name C)	(segid 3A4 and resid 155 and name O)	1.23	0.00	0.00
	assign (segid 3A4 and resid 155 and name C)	(segid 3A4 and resid 156 and name C)	3.03	0.07	0.06
5	assign (segid 3A4 and resid 155 and name C)	(segid 3A4 and resid 156 and name CA)	2.44	0.02	0.03
	assign (segid 3A4 and resid 155 and name C)	(segid 3A4 and resid 156 and name CB)	3.71	0.04	0.03
	assign (segid 3A4 and resid 155 and name C)	(segid 3A4 and resid 156 and name N)	1.33	0.00	0.01
	assign (segid 3A4 and resid 155 and name C)	(segid 3A4 and resid 156 and name O)	3.83	0.07	0.06
	assign (segid 3A4 and resid 155 and name C)	(segid 3A4 and resid 157 and name C)	4.60	0.13	0.12
10	assign (segid 3A4 and resid 155 and name C)	(segid 3A4 and resid 157 and name CA)	4.49	0.14	0.15
	assign (segid 3A4 and resid 155 and name C)	(segid 3A4 and resid 157 and name CB)	5.28	0.25	0.24
	assign (segid 3A4 and resid 155 and name C)	(segid 3A4 and resid 157 and name N)	3.31	0.13	0.13
	assign (segid 3A4 and resid 155 and name C)	(segid 3A4 and resid 157 and name O)	5.66	0.12	0.11
	assign (segid 3A4 and resid 155 and name C)	(segid 3A4 and resid 158 and name C)	4.96	0.14	0.13
15	assign (segid 3A4 and resid 155 and name C)	(segid 3A4 and resid 158 and name CA)	4.65	0.18	0.18
	assign (segid 3A4 and resid 155 and name C)	(segid 3A4 and resid 158 and name CB)	4.52	0.36	0.35
	assign (segid 3A4 and resid 155 and name C)	(segid 3A4 and resid 158 and name N)	3.90	0.16	0.16
	assign (segid 3A4 and resid 155 and name C)	(segid 3A4 and resid 158 and name O)	6.14	0.16	0.16
	assign (segid 3A4 and resid 155 and name C)	(segid 3A4 and resid 159 and name C)	6.08	0.51	0.51
20	assign (segid 3A4 and resid 155 and name C)	(segid 3A4 and resid 159 and name CA)	5.09	0.30	0.29
	assign (segid 3A4 and resid 155 and name C)	(segid 3A4 and resid 159 and name CB)	4.74	0.29	0.29
	assign (segid 3A4 and resid 155 and name C)	(segid 3A4 and resid 159 and name N)	4.21	0.21	0.20
	assign (segid 3A4 and resid 155 and name C)	(segid 3A4 and resid 159 and name O)	7.23	0.49	0.50
	assign (segid 3A4 and resid 155 and name C)	(segid 3A4 and resid 160 and name CA)	7.15	0.77	0.78
25	assign (segid 3A4 and resid 155 and name C)	(segid 3A4 and resid 160 and name CB)	7.17	0.92	0.91
	assign (segid 3A4 and resid 155 and name C)	(segid 3A4 and resid 160 and name N)	5.90	0.69	0.68
	assign (segid 3A4 and resid 155 and name C)	(segid 3A4 and resid 160 and name O)	1.53	0.00	0.01
	assign (segid 3A4 and resid 155 and name CA)	(segid 3A4 and resid 155 and name CB)	1.54	0.01	0.00
	assign (segid 3A4 and resid 155 and name CA)	(segid 3A4 and resid 155 and name O)	2.40	0.02	0.02
30	assign (segid 3A4 and resid 155 and name CA)	(segid 3A4 and resid 156 and name C)	4.44	0.05	0.05
	assign (segid 3A4 and resid 155 and name CA)	(segid 3A4 and resid 156 and name CA)	3.82	0.02	0.03
	assign (segid 3A4 and resid 155 and name CA)	(segid 3A4 and resid 156 and name CB)	4.85	0.06	0.06
	assign (segid 3A4 and resid 155 and name CA)	(segid 3A4 and resid 156 and name N)	2.44	0.02	0.01
	assign (segid 3A4 and resid 155 and name CA)	(segid 3A4 and resid 156 and name O)	5.31	0.06	0.06
35	assign (segid 3A4 and resid 155 and name CA)	(segid 3A4 and resid 157 and name C)	5.57	0.10	0.10
	assign (segid 3A4 and resid 155 and name CA)	(segid 3A4 and resid 157 and name CA)	5.52	0.14	0.14
	assign (segid 3A4 and resid 155 and name CA)	(segid 3A4 and resid 157 and name CB)	5.99	0.29	0.30
	assign (segid 3A4 and resid 155 and name CA)	(segid 3A4 and resid 157 and name N)	4.45	0.11	0.11
	assign (segid 3A4 and resid 155 and name CA)	(segid 3A4 and resid 157 and name O)	6.69	0.10	0.09
40	assign (segid 3A4 and resid 155 and name CA)	(segid 3A4 and resid 158 and name C)	5.76	0.21	0.21
	assign (segid 3A4 and resid 155 and name CA)	(segid 3A4 and resid 158 and name CA)	5.24	0.13	0.14
	assign (segid 3A4 and resid 155 and name CA)	(segid 3A4 and resid 158 and name CB)	4.70	0.29	0.29
	assign (segid 3A4 and resid 155 and name CA)	(segid 3A4 and resid 158 and name N)	4.66	0.12	0.12
	assign (segid 3A4 and resid 155 and name CA)	(segid 3A4 and resid 158 and name O)	6.92	0.23	0.23
45	assign (segid 3A4 and resid 155 and name CA)	(segid 3A4 and resid 159 and name C)	7.26	0.65	0.66
	assign (segid 3A4 and resid 155 and name CA)	(segid 3A4 and resid 159 and name CA)	6.13	0.50	0.50
	assign (segid 3A4 and resid 155 and name CA)	(segid 3A4 and resid 159 and name CB)	5.80	0.61	0.61
	assign (segid 3A4 and resid 155 and name CA)	(segid 3A4 and resid 159 and name N)	5.18	0.36	0.36
	assign (segid 3A4 and resid 155 and name CA)	(segid 3A4 and resid 160 and name CA)	8.49	0.84	0.83
50	assign (segid 3A4 and resid 155 and name CA)	(segid 3A4 and resid 160 and name CB)	8.54	0.94	0.95
	assign (segid 3A4 and resid 155 and name CA)	(segid 3A4 and resid 160 and name N)	7.19	0.78	0.78
	assign (segid 3A4 and resid 155 and name CA)	(segid 3A4 and resid 161 and name CA)	9.90	0.59	0.60
	assign (segid 3A4 and resid 155 and name CA)	(segid 3A4 and resid 161 and name CB)	9.72	0.52	0.52
	assign (segid 3A4 and resid 155 and name CA)	(segid 3A4 and resid 187 and name CA)	10.40	2.12	2.13
55	assign (segid 3A4 and resid 155 and name CA)	(segid 3A4 and resid 187 and name CB)	11.22	2.29	2.29
	assign (segid 3A4 and resid 155 and name CA)	(segid 3A4 and resid 188 and name CA)	12.69	1.99	1.98
	assign (segid 3A4 and resid 155 and name CA)	(segid 3A4 and resid 189 and name CA)	11.48	1.69	1.69
	assign (segid 3A4 and resid 155 and name CA)	(segid 3A4 and resid 189 and name CB)	11.56	1.75	1.76
	assign (segid 3A4 and resid 155 and name CA)	(segid 3A4 and resid 190 and name CA)	8.04	1.60	1.60
60	assign (segid 3A4 and resid 155 and name CA)	(segid 3A4 and resid 190 and name CB)	7.13	1.65	1.65
	assign (segid 3A4 and resid 155 and name CA)	(segid 3A4 and resid 191 and name CA)	9.99	1.66	1.66
	assign (segid 3A4 and resid 155 and name CA)	(segid 3A4 and resid 191 and name CB)	11.00	1.82	1.81
	assign (segid 3A4 and resid 155 and name CA)	(segid 3A4 and resid 192 and name CA)	12.30	1.50	1.50
	assign (segid 3A4 and resid 155 and name CA)	(segid 3A4 and resid 192 and name CB)	13.12	1.59	1.60
65	assign (segid 3A4 and resid 155 and name CA)	(segid 3A4 and resid 193 and name CA)	10.31	1.21	1.22
	assign (segid 3A4 and resid 155 and name CA)	(segid 3A4 and resid 193 and name CB)	9.28	1.26	1.25
	assign (segid 3A4 and resid 155 and name CA)	(segid 3A4 and resid 194 and name CA)	9.52	1.01	1.01
	assign (segid 3A4 and resid 155 and name CA)	(segid 3A4 and resid 194 and name CB)	8.90	1.00	0.99
	assign (segid 3A4 and resid 155 and name CA)	(segid 3A4 and resid 195 and name CA)	13.02	1.12	1.11
70	assign (segid 3A4 and resid 155 and name CA)	(segid 3A4 and resid 195 and name CB)	13.70	1.27	1.26
	assign (segid 3A4 and resid 155 and name CA)	(segid 3A4 and resid 196 and name CA)	14.28	1.03	1.03
	assign (segid 3A4 and resid 155 and name CA)	(segid 3A4 and resid 196 and name CB)	14.12	1.07	1.07
	assign (segid 3A4 and resid 155 and name CA)	(segid 3A4 and resid 197 and name CA)	13.03	1.04	1.04
	assign (segid 3A4 and resid 155 and name CA)	(segid 3A4 and resid 197 and name CB)	11.71	1.17	1.16
75	assign (segid 3A4 and resid 155 and name CA)	(segid 3A4 and resid 198 and name CA)	14.55	0.85	0.86
	assign (segid 3A4 and resid 155 and name CA)	(segid 3A4 and resid 198 and name CB)	14.23	0.84	0.84
	assign (segid 3A4 and resid 155 and name CA)	(segid 3A4 and resid 199 and name CA)	17.53	0.88	0.89
	assign (segid 3A4 and resid 155 and name CA)	(segid 3A4 and resid 199 and name CB)	17.66	0.95	0.94
80	assign (segid 3A4 and resid 155 and name CA)	(segid 3A4 and resid 200 and name CA)	18.41	1.04	1.04
	assign (segid 3A4 and resid 155 and name CA)	(segid 3A4 and resid 201 and name CB)	17.28	0.89	0.90
	assign (segid 3A4 and resid 155 and name CA)	(segid 3A4 and resid 248 and name CA)	16.04	1.30	1.30
	assign (segid 3A4 and resid 155 and name CA)	(segid 3A4 and resid 248 and name CB)	16.09	1.38	1.39

	assign (segid 3A4 and resid 155 and name CA)	(segid 3A4 and resid 249 and name CA)	13.12	1.42	1.41
	assign (segid 3A4 and resid 155 and name CA)	(segid 3A4 and resid 250 and name CA)	14.70	1.30	1.30
	assign (segid 3A4 and resid 155 and name CA)	(segid 3A4 and resid 250 and name CB)	16.05	1.37	1.38
	assign (segid 3A4 and resid 155 and name CA)	(segid 3A4 and resid 251 and name CA)	15.51	0.83	0.83
5	assign (segid 3A4 and resid 155 and name CA)	(segid 3A4 and resid 251 and name CB)	16.39	0.86	0.85
	assign (segid 3A4 and resid 155 and name CA)	(segid 3A4 and resid 252 and name CA)	12.19	0.78	0.78
	assign (segid 3A4 and resid 155 and name CA)	(segid 3A4 and resid 252 and name CB)	11.41	0.89	0.89
	assign (segid 3A4 and resid 155 and name CA)	(segid 3A4 and resid 253 and name CA)	10.91	0.86	0.85
	assign (segid 3A4 and resid 155 and name CA)	(segid 3A4 and resid 254 and name CA)	14.23	0.82	0.82
10	assign (segid 3A4 and resid 155 and name CA)	(segid 3A4 and resid 255 and name CA)	14.73	0.72	0.71
	assign (segid 3A4 and resid 155 and name CA)	(segid 3A4 and resid 256 and name CA)	12.14	1.14	1.15
	assign (segid 3A4 and resid 155 and name CA)	(segid 3A4 and resid 257 and name CA)	12.05	1.07	1.07
	assign (segid 3A4 and resid 155 and name CA)	(segid 3A4 and resid 258 and name CA)	15.55	0.84	0.84
	assign (segid 3A4 and resid 155 and name CA)	(segid 3A4 and resid 258 and name CB)	16.29	0.62	0.62
15	assign (segid 3A4 and resid 155 and name CA)	(segid 3A4 and resid 259 and name CA)	16.75	1.09	1.08
	assign (segid 3A4 and resid 155 and name CA)	(segid 3A4 and resid 259 and name CB)	16.73	1.15	1.16
	assign (segid 3A4 and resid 155 and name CA)	(segid 3A4 and resid 260 and name CA)	14.97	1.67	1.67
	assign (segid 3A4 and resid 155 and name CA)	(segid 3A4 and resid 260 and name CB)	13.61	1.79	1.79
	assign (segid 3A4 and resid 155 and name CA)	(segid 3A4 and resid 261 and name CA)	16.36	1.36	1.37
20	assign (segid 3A4 and resid 155 and name CA)	(segid 3A4 and resid 434 and name CA)	17.29	1.73	1.72
	assign (segid 3A4 and resid 155 and name CB)	(segid 3A4 and resid 156 and name C)	5.44	0.09	0.09
	assign (segid 3A4 and resid 155 and name CB)	(segid 3A4 and resid 156 and name CA)	4.47	0.07	0.08
	assign (segid 3A4 and resid 155 and name CB)	(segid 3A4 and resid 156 and name CB)	5.32	0.12	0.12
	assign (segid 3A4 and resid 155 and name CB)	(segid 3A4 and resid 156 and name N)	3.14	0.09	0.10
25	assign (segid 3A4 and resid 155 and name CB)	(segid 3A4 and resid 156 and name O)	6.27	0.09	0.08
	assign (segid 3A4 and resid 155 and name CB)	(segid 3A4 and resid 157 and name C)	6.98	0.11	0.11
	assign (segid 3A4 and resid 155 and name CB)	(segid 3A4 and resid 157 and name CA)	6.87	0.15	0.15
	assign (segid 3A4 and resid 155 and name CB)	(segid 3A4 and resid 157 and name CB)	7.40	0.28	0.28
	assign (segid 3A4 and resid 155 and name CB)	(segid 3A4 and resid 157 and name N)	5.67	0.14	0.13
30	assign (segid 3A4 and resid 155 and name CB)	(segid 3A4 and resid 158 and name C)	6.95	0.16	0.17
	assign (segid 3A4 and resid 155 and name CB)	(segid 3A4 and resid 158 and name CA)	6.61	0.18	0.17
	assign (segid 3A4 and resid 155 and name CB)	(segid 3A4 and resid 158 and name CB)	5.98	0.37	0.38
	assign (segid 3A4 and resid 155 and name CB)	(segid 3A4 and resid 158 and name N)	6.10	0.14	0.14
	assign (segid 3A4 and resid 155 and name CB)	(segid 3A4 and resid 159 and name CA)	6.96	0.44	0.43
35	assign (segid 3A4 and resid 155 and name CB)	(segid 3A4 and resid 159 and name CB)	6.36	0.56	0.57
	assign (segid 3A4 and resid 155 and name CB)	(segid 3A4 and resid 159 and name N)	6.23	0.28	0.28
	assign (segid 3A4 and resid 155 and name CB)	(segid 3A4 and resid 160 and name CA)	9.44	0.96	0.96
	assign (segid 3A4 and resid 155 and name CB)	(segid 3A4 and resid 160 and name CB)	9.50	1.17	1.16
	assign (segid 3A4 and resid 155 and name CB)	(segid 3A4 and resid 161 and name CA)	11.12	0.66	0.65
40	assign (segid 3A4 and resid 155 and name CB)	(segid 3A4 and resid 161 and name CB)	11.01	0.59	0.59
	assign (segid 3A4 and resid 155 and name CB)	(segid 3A4 and resid 167 and name CA)	10.65	2.16	2.15
	assign (segid 3A4 and resid 155 and name CB)	(segid 3A4 and resid 167 and name CB)	11.56	2.31	2.32
	assign (segid 3A4 and resid 155 and name CB)	(segid 3A4 and resid 168 and name CA)	12.64	2.17	2.18
	assign (segid 3A4 and resid 155 and name CB)	(segid 3A4 and resid 169 and name CA)	11.18	1.76	1.76
45	assign (segid 3A4 and resid 155 and name CB)	(segid 3A4 and resid 169 and name CB)	11.25	1.69	1.68
	assign (segid 3A4 and resid 155 and name CB)	(segid 3A4 and resid 190 and name CA)	7.86	1.79	1.78
	assign (segid 3A4 and resid 155 and name CB)	(segid 3A4 and resid 190 and name CB)	7.15	1.78	1.77
	assign (segid 3A4 and resid 155 and name CB)	(segid 3A4 and resid 191 and name CA)	9.86	2.22	2.22
	assign (segid 3A4 and resid 155 and name CB)	(segid 3A4 and resid 191 and name CB)	10.95	2.37	2.38
50	assign (segid 3A4 and resid 155 and name CB)	(segid 3A4 and resid 191 and name CA)	11.91	1.96	1.96
	assign (segid 3A4 and resid 155 and name CB)	(segid 3A4 and resid 192 and name CB)	12.71	1.99	1.98
	assign (segid 3A4 and resid 155 and name CB)	(segid 3A4 and resid 192 and name CA)	9.73	1.56	1.57
	assign (segid 3A4 and resid 155 and name CB)	(segid 3A4 and resid 193 and name CB)	8.68	1.50	1.50
	assign (segid 3A4 and resid 155 and name CB)	(segid 3A4 and resid 193 and name CA)	9.17	1.61	1.61
55	assign (segid 3A4 and resid 155 and name CB)	(segid 3A4 and resid 194 and name CB)	8.70	1.68	1.69
	assign (segid 3A4 and resid 155 and name CB)	(segid 3A4 and resid 195 and name CA)	12.67	1.78	1.78
	assign (segid 3A4 and resid 155 and name CB)	(segid 3A4 and resid 195 and name CB)	13.38	1.94	1.93
	assign (segid 3A4 and resid 155 and name CB)	(segid 3A4 and resid 196 and name CA)	13.70	1.49	1.48
	assign (segid 3A4 and resid 155 and name CB)	(segid 3A4 and resid 196 and name CB)	13.47	1.45	1.44
60	assign (segid 3A4 and resid 155 and name CB)	(segid 3A4 and resid 197 and name CA)	12.49	1.31	1.31
	assign (segid 3A4 and resid 155 and name CB)	(segid 3A4 and resid 197 and name CB)	11.21	1.35	1.35
	assign (segid 3A4 and resid 155 and name CB)	(segid 3A4 and resid 198 and name CA)	14.23	1.37	1.37
	assign (segid 3A4 and resid 155 and name CB)	(segid 3A4 and resid 198 and name CB)	13.99	1.48	1.48
	assign (segid 3A4 and resid 155 and name CB)	(segid 3A4 and resid 199 and name CA)	17.09	1.49	1.48
65	assign (segid 3A4 and resid 155 and name CB)	(segid 3A4 and resid 199 and name CB)	17.18	1.57	1.56
	assign (segid 3A4 and resid 155 and name CB)	(segid 3A4 and resid 200 and name CA)	17.85	1.37	1.36
	assign (segid 3A4 and resid 155 and name CB)	(segid 3A4 and resid 201 and name CA)	17.96	1.01	1.00
	assign (segid 3A4 and resid 155 and name CB)	(segid 3A4 and resid 201 and name CB)	16.95	0.92	0.91
	assign (segid 3A4 and resid 155 and name CB)	(segid 3A4 and resid 248 and name CA)	16.23	1.97	1.96
	assign (segid 3A4 and resid 155 and name CB)	(segid 3A4 and resid 248 and name CB)	16.18	2.00	2.01
70	assign (segid 3A4 and resid 155 and name CB)	(segid 3A4 and resid 249 and name CA)	13.38	2.13	2.12
	assign (segid 3A4 and resid 155 and name CB)	(segid 3A4 and resid 250 and name CA)	15.22	2.01	2.01
	assign (segid 3A4 and resid 155 and name CB)	(segid 3A4 and resid 251 and name CA)	16.07	1.46	1.45
	assign (segid 3A4 and resid 155 and name CB)	(segid 3A4 and resid 251 and name CB)	16.87	1.46	1.45
	assign (segid 3A4 and resid 155 and name CB)	(segid 3A4 and resid 252 and name CA)	12.75	1.22	1.23
75	assign (segid 3A4 and resid 155 and name CB)	(segid 3A4 and resid 252 and name CB)	11.87	1.35	1.35
	assign (segid 3A4 and resid 155 and name CB)	(segid 3A4 and resid 253 and name CA)	11.70	1.38	1.39
	assign (segid 3A4 and resid 155 and name CB)	(segid 3A4 and resid 254 and name CA)	15.12	1.33	1.32
	assign (segid 3A4 and resid 155 and name CB)	(segid 3A4 and resid 255 and name CA)	15.56	0.89	0.90
	assign (segid 3A4 and resid 155 and name CB)	(segid 3A4 and resid 256 and name CA)	13.07	0.96	0.97
80	assign (segid 3A4 and resid 155 and name CB)	(segid 3A4 and resid 257 and name CA)	13.18	0.86	0.86
	assign (segid 3A4 and resid 155 and name CB)	(segid 3A4 and resid 258 and name CA)	16.66	0.71	0.70
	assign (segid 3A4 and resid 155 and name CB)	(segid 3A4 and resid 258 and name CB)	17.36	0.64	0.65

	assign (segid 3A4 and resid 155 and name CB)	(segid 3A4 and resid 259 and name CA)	17.76	0.77	0.76
	assign (segid 3A4 and resid 155 and name CB)	(segid 3A4 and resid 259 and name CB)	17.69	0.84	0.83
	assign (segid 3A4 and resid 155 and name CB)	(segid 3A4 and resid 260 and name CA)	16.00	1.40	1.39
	assign (segid 3A4 and resid 155 and name CB)	(segid 3A4 and resid 260 and name CB)	14.65	1.51	1.51
5	assign (segid 3A4 and resid 155 and name CB)	(segid 3A4 and resid 261 and name CA)	17.48	1.19	1.20
	assign (segid 3A4 and resid 155 and name N)	(segid 3A4 and resid 155 and name C)	2.47	0.03	0.02
	assign (segid 3A4 and resid 155 and name N)	(segid 3A4 and resid 155 and name CA)	1.46	0.01	0.00
	assign (segid 3A4 and resid 155 and name N)	(segid 3A4 and resid 155 and name CB)	2.46	0.03	0.02
	assign (segid 3A4 and resid 155 and name N)	(segid 3A4 and resid 155 and name O)	3.48	0.05	0.05
10	assign (segid 3A4 and resid 155 and name N)	(segid 3A4 and resid 156 and name C)	4.77	0.04	0.04
	assign (segid 3A4 and resid 155 and name N)	(segid 3A4 and resid 156 and name CA)	4.24	0.07	0.07
	assign (segid 3A4 and resid 155 and name N)	(segid 3A4 and resid 156 and name CB)	4.96	0.11	0.11
	assign (segid 3A4 and resid 155 and name N)	(segid 3A4 and resid 156 and name N)	2.84	0.08	0.08
	assign (segid 3A4 and resid 155 and name N)	(segid 3A4 and resid 156 and name O)	5.82	0.05	0.05
15	assign (segid 3A4 and resid 155 and name N)	(segid 3A4 and resid 157 and name C)	5.69	0.10	0.09
	assign (segid 3A4 and resid 155 and name N)	(segid 3A4 and resid 157 and name CA)	5.41	0.13	0.13
	assign (segid 3A4 and resid 155 and name N)	(segid 3A4 and resid 157 and name CB)	5.52	0.30	0.30
	assign (segid 3A4 and resid 155 and name N)	(segid 3A4 and resid 157 and name N)	4.41	0.09	0.08
	assign (segid 3A4 and resid 155 and name N)	(segid 3A4 and resid 157 and name O)	6.89	0.10	0.09
20	assign (segid 3A4 and resid 155 and name N)	(segid 3A4 and resid 158 and name C)	6.45	0.30	0.29
	assign (segid 3A4 and resid 155 and name N)	(segid 3A4 and resid 158 and name CA)	5.65	0.12	0.12
	assign (segid 3A4 and resid 155 and name N)	(segid 3A4 and resid 158 and name CB)	5.14	0.12	0.12
	assign (segid 3A4 and resid 155 and name N)	(segid 3A4 and resid 158 and name N)	4.87	0.09	0.09
	assign (segid 3A4 and resid 155 and name N)	(segid 3A4 and resid 159 and name CA)	7.15	0.52	0.52
25	assign (segid 3A4 and resid 155 and name N)	(segid 3A4 and resid 159 and name CB)	6.95	0.60	0.60
	assign (segid 3A4 and resid 155 and name N)	(segid 3A4 and resid 159 and name N)	6.04	0.43	0.44
	assign (segid 3A4 and resid 155 and name O)	(segid 3A4 and resid 155 and name CB)	3.33	0.07	0.08
	assign (segid 3A4 and resid 155 and name O)	(segid 3A4 and resid 156 and name C)	2.95	0.12	0.12
	assign (segid 3A4 and resid 155 and name O)	(segid 3A4 and resid 156 and name CA)	2.79	0.03	0.02
30	assign (segid 3A4 and resid 155 and name O)	(segid 3A4 and resid 156 and name CB)	4.26	0.03	0.03
	assign (segid 3A4 and resid 155 and name O)	(segid 3A4 and resid 156 and name N)	2.25	0.01	0.02
	assign (segid 3A4 and resid 155 and name O)	(segid 3A4 and resid 157 and name C)	3.38	0.10	0.10
	assign (segid 3A4 and resid 155 and name O)	(segid 3A4 and resid 157 and name CA)	4.13	0.24	0.24
	assign (segid 3A4 and resid 155 and name O)	(segid 3A4 and resid 157 and name CB)	4.37	0.26	0.26
35	assign (segid 3A4 and resid 155 and name O)	(segid 3A4 and resid 157 and name N)	5.38	0.31	0.31
	assign (segid 3A4 and resid 155 and name O)	(segid 3A4 and resid 157 and name O)	3.42	0.23	0.23
	assign (segid 3A4 and resid 155 and name O)	(segid 3A4 and resid 158 and name C)	5.04	0.22	0.22
	assign (segid 3A4 and resid 155 and name O)	(segid 3A4 and resid 158 and name CA)	3.94	0.15	0.15
	assign (segid 3A4 and resid 155 and name O)	(segid 3A4 and resid 158 and name CB)	3.89	0.25	0.26
40	assign (segid 3A4 and resid 155 and name O)	(segid 3A4 and resid 158 and name N)	3.86	0.47	0.48
	assign (segid 3A4 and resid 155 and name O)	(segid 3A4 and resid 158 and name O)	3.38	0.25	0.25
	assign (segid 3A4 and resid 155 and name O)	(segid 3A4 and resid 159 and name C)	5.08	0.16	0.16
	assign (segid 3A4 and resid 155 and name O)	(segid 3A4 and resid 159 and name CA)	4.97	0.56	0.56
	assign (segid 3A4 and resid 155 and name O)	(segid 3A4 and resid 159 and name CB)	3.95	0.28	0.28
45	assign (segid 3A4 and resid 155 and name O)	(segid 3A4 and resid 159 and name N)	3.72	0.26	0.26
	assign (segid 3A4 and resid 155 and name O)	(segid 3A4 and resid 159 and name O)	3.11	0.18	0.18
	assign (segid 3A4 and resid 155 and name O)	(segid 3A4 and resid 160 and name C)	6.10	0.54	0.54
	assign (segid 3A4 and resid 155 and name O)	(segid 3A4 and resid 160 and name CA)	7.11	0.85	0.84
	assign (segid 3A4 and resid 155 and name O)	(segid 3A4 and resid 160 and name CB)	6.24	0.87	0.86
50	assign (segid 3A4 and resid 155 and name O)	(segid 3A4 and resid 160 and name N)	6.45	0.99	0.99
	assign (segid 3A4 and resid 155 and name O)	(segid 3A4 and resid 161 and name N)	4.91	0.78	0.78
	assign (segid 3A4 and resid 156 and name C)	(segid 3A4 and resid 156 and name CB)	6.77	0.79	0.78
	assign (segid 3A4 and resid 156 and name C)	(segid 3A4 and resid 156 and name O)	2.51	0.03	0.03
	assign (segid 3A4 and resid 156 and name C)	(segid 3A4 and resid 156 and name O)	1.24	0.00	0.00
	assign (segid 3A4 and resid 156 and name C)	(segid 3A4 and resid 157 and name C)	3.07	0.07	0.07
55	assign (segid 3A4 and resid 156 and name C)	(segid 3A4 and resid 157 and name CA)	2.44	0.01	0.02
	assign (segid 3A4 and resid 156 and name C)	(segid 3A4 and resid 157 and name CB)	3.72	0.03	0.03
	assign (segid 3A4 and resid 156 and name C)	(segid 3A4 and resid 157 and name N)	1.33	0.01	0.01
	assign (segid 3A4 and resid 156 and name C)	(segid 3A4 and resid 157 and name O)	3.89	0.06	0.06
	assign (segid 3A4 and resid 156 and name C)	(segid 3A4 and resid 158 and name C)	4.66	0.17	0.17
60	assign (segid 3A4 and resid 156 and name C)	(segid 3A4 and resid 158 and name CA)	4.55	0.17	0.17
	assign (segid 3A4 and resid 156 and name C)	(segid 3A4 and resid 158 and name CB)	5.32	0.25	0.24
	assign (segid 3A4 and resid 156 and name C)	(segid 3A4 and resid 158 and name N)	3.36	0.16	0.15
	assign (segid 3A4 and resid 156 and name C)	(segid 3A4 and resid 158 and name O)	5.69	0.12	0.12
	assign (segid 3A4 and resid 156 and name C)	(segid 3A4 and resid 159 and name C)	5.04	0.09	0.09
65	assign (segid 3A4 and resid 156 and name C)	(segid 3A4 and resid 159 and name CA)	4.71	0.28	0.29
	assign (segid 3A4 and resid 156 and name C)	(segid 3A4 and resid 159 and name CB)	4.59	0.50	0.51
	assign (segid 3A4 and resid 156 and name C)	(segid 3A4 and resid 159 and name N)	3.97	0.26	0.26
	assign (segid 3A4 and resid 156 and name C)	(segid 3A4 and resid 159 and name O)	6.18	0.09	0.09
	assign (segid 3A4 and resid 156 and name C)	(segid 3A4 and resid 160 and name C)	6.21	0.49	0.50
70	assign (segid 3A4 and resid 156 and name C)	(segid 3A4 and resid 160 and name CA)	5.27	0.20	0.21
	assign (segid 3A4 and resid 156 and name C)	(segid 3A4 and resid 160 and name CB)	4.96	0.26	0.25
	assign (segid 3A4 and resid 156 and name C)	(segid 3A4 and resid 160 and name N)	4.38	0.09	0.09
	assign (segid 3A4 and resid 156 and name C)	(segid 3A4 and resid 160 and name O)	7.37	0.49	0.48
	assign (segid 3A4 and resid 156 and name C)	(segid 3A4 and resid 161 and name N)	5.99	0.73	0.72
75	assign (segid 3A4 and resid 156 and name C)	(segid 3A4 and resid 156 and name C)	1.52	0.01	0.01
	assign (segid 3A4 and resid 156 and name CA)	(segid 3A4 and resid 156 and name CB)	1.53	0.01	0.01
	assign (segid 3A4 and resid 156 and name CA)	(segid 3A4 and resid 156 and name O)	2.40	0.03	0.03
	assign (segid 3A4 and resid 156 and name CA)	(segid 3A4 and resid 157 and name C)	4.45	0.08	0.08
80	assign (segid 3A4 and resid 156 and name CA)	(segid 3A4 and resid 157 and name CA)	3.79	0.02	0.02
	assign (segid 3A4 and resid 156 and name CA)	(segid 3A4 and resid 157 and name CB)	4.83	0.07	0.07
	assign (segid 3A4 and resid 156 and name CA)	(segid 3A4 and resid 157 and name N)	2.41	0.03	0.03
	assign (segid 3A4 and resid 156 and name CA)	(segid 3A4 and resid 157 and name O)	5.36	0.07	0.07

5	assign	(segid 3A4 and resid 156 and name CA)	(segid 3A4 and resid 158 and name C)	5.65	0.18	0.18
	assign	(segid 3A4 and resid 156 and name CA)	(segid 3A4 and resid 158 and name CA)	5.56	0.20	0.20
	assign	(segid 3A4 and resid 156 and name CA)	(segid 3A4 and resid 158 and name CB)	6.01	0.30	0.31
	assign	(segid 3A4 and resid 156 and name CA)	(segid 3A4 and resid 158 and name N)	4.46	0.17	0.16
	assign	(segid 3A4 and resid 156 and name CA)	(segid 3A4 and resid 158 and name O)	6.75	0.14	0.13
	assign	(segid 3A4 and resid 156 and name CA)	(segid 3A4 and resid 159 and name C)	5.91	0.13	0.13
	assign	(segid 3A4 and resid 156 and name CA)	(segid 3A4 and resid 159 and name CA)	5.38	0.24	0.24
	assign	(segid 3A4 and resid 156 and name CA)	(segid 3A4 and resid 159 and name CB)	4.88	0.45	0.44
	assign	(segid 3A4 and resid 156 and name CA)	(segid 3A4 and resid 159 and name N)	4.77	0.23	0.23
	assign	(segid 3A4 and resid 156 and name CA)	(segid 3A4 and resid 159 and name O)	7.05	0.18	0.18
10	assign	(segid 3A4 and resid 156 and name CA)	(segid 3A4 and resid 160 and name CA)	6.34	0.47	0.48
	assign	(segid 3A4 and resid 156 and name CA)	(segid 3A4 and resid 160 and name CB)	6.01	0.64	0.65
	assign	(segid 3A4 and resid 156 and name CA)	(segid 3A4 and resid 160 and name N)	5.39	0.28	0.28
	assign	(segid 3A4 and resid 156 and name CA)	(segid 3A4 and resid 161 and name CA)	8.54	0.93	0.93
	assign	(segid 3A4 and resid 156 and name CA)	(segid 3A4 and resid 161 and name CB)	8.57	1.09	1.08
15	assign	(segid 3A4 and resid 156 and name CA)	(segid 3A4 and resid 167 and name CA)	9.49	1.01	1.02
	assign	(segid 3A4 and resid 156 and name CA)	(segid 3A4 and resid 167 and name CB)	10.18	1.02	1.02
	assign	(segid 3A4 and resid 156 and name CA)	(segid 3A4 and resid 168 and name CA)	11.52	1.04	1.04
	assign	(segid 3A4 and resid 156 and name CA)	(segid 3A4 and resid 169 and name CA)	10.72	1.55	1.56
20	assign	(segid 3A4 and resid 156 and name CA)	(segid 3A4 and resid 169 and name CB)	11.08	1.81	1.80
	assign	(segid 3A4 and resid 156 and name CA)	(segid 3A4 and resid 190 and name CA)	7.11	1.59	1.59
	assign	(segid 3A4 and resid 156 and name CA)	(segid 3A4 and resid 190 and name CB)	6.26	1.49	1.49
	assign	(segid 3A4 and resid 156 and name CA)	(segid 3A4 and resid 191 and name CA)	8.34	0.84	0.84
	assign	(segid 3A4 and resid 156 and name CA)	(segid 3A4 and resid 191 and name CB)	9.27	0.56	0.56
25	assign	(segid 3A4 and resid 156 and name CA)	(segid 3A4 and resid 192 and name CA)	10.96	1.28	1.27
	assign	(segid 3A4 and resid 156 and name CA)	(segid 3A4 and resid 192 and name CB)	11.94	1.26	1.26
	assign	(segid 3A4 and resid 156 and name CA)	(segid 3A4 and resid 193 and name CA)	9.36	1.79	1.78
	assign	(segid 3A4 and resid 156 and name CA)	(segid 3A4 and resid 193 and name CB)	8.54	1.96	1.95
	assign	(segid 3A4 and resid 156 and name CA)	(segid 3A4 and resid 194 and name CA)	8.02	1.40	1.40
30	assign	(segid 3A4 and resid 156 and name CA)	(segid 3A4 and resid 194 and name CB)	7.16	1.22	1.22
	assign	(segid 3A4 and resid 156 and name CA)	(segid 3A4 and resid 195 and name CA)	11.32	1.12	1.12
	assign	(segid 3A4 and resid 156 and name CA)	(segid 3A4 and resid 195 and name CB)	11.95	1.00	1.00
	assign	(segid 3A4 and resid 156 and name CA)	(segid 3A4 and resid 196 and name CA)	13.10	1.57	1.57
	assign	(segid 3A4 and resid 156 and name CA)	(segid 3A4 and resid 196 and name CB)	13.13	1.71	1.72
35	assign	(segid 3A4 and resid 156 and name CA)	(segid 3A4 and resid 197 and name CA)	12.09	1.83	1.83
	assign	(segid 3A4 and resid 156 and name CA)	(segid 3A4 and resid 197 and name CB)	10.82	1.98	1.98
	assign	(segid 3A4 and resid 156 and name CA)	(segid 3A4 and resid 198 and name CA)	13.11	1.40	1.39
	assign	(segid 3A4 and resid 156 and name CA)	(segid 3A4 and resid 198 and name CB)	12.56	1.23	1.23
	assign	(segid 3A4 and resid 156 and name CA)	(segid 3A4 and resid 199 and name CA)	16.08	1.21	1.22
40	assign	(segid 3A4 and resid 156 and name CA)	(segid 3A4 and resid 199 and name CB)	16.21	1.15	1.15
	assign	(segid 3A4 and resid 156 and name CA)	(segid 3A4 and resid 245 and name CA)	15.45	1.44	1.43
	assign	(segid 3A4 and resid 156 and name CA)	(segid 3A4 and resid 245 and name CB)	15.44	1.47	1.46
	assign	(segid 3A4 and resid 156 and name CA)	(segid 3A4 and resid 246 and name CA)	14.67	1.45	1.44
	assign	(segid 3A4 and resid 156 and name CA)	(segid 3A4 and resid 246 and name CB)	15.61	1.48	1.47
45	assign	(segid 3A4 and resid 156 and name CA)	(segid 3A4 and resid 247 and name CA)	15.81	1.50	1.50
	assign	(segid 3A4 and resid 156 and name CA)	(segid 3A4 and resid 247 and name CB)	17.18	1.52	1.51
	assign	(segid 3A4 and resid 156 and name CA)	(segid 3A4 and resid 248 and name CA)	13.85	1.57	1.58
	assign	(segid 3A4 and resid 156 and name CA)	(segid 3A4 and resid 248 and name CB)	14.05	1.66	1.66

	assign (segid 3A4 and resid 156 and name CB)	(segid 3A4 and resid 160 and name CB)	6.67	0.50	0.50
	assign (segid 3A4 and resid 156 and name CB)	(segid 3A4 and resid 160 and name N)	6.48	0.15	0.15
	assign (segid 3A4 and resid 156 and name CB)	(segid 3A4 and resid 161 and name CA)	9.54	0.97	0.98
	assign (segid 3A4 and resid 156 and name CB)	(segid 3A4 and resid 161 and name CB)	9.54	1.22	1.21
5	assign (segid 3A4 and resid 156 and name CB)	(segid 3A4 and resid 187 and name CA)	10.23	1.13	1.14
	assign (segid 3A4 and resid 156 and name CB)	(segid 3A4 and resid 187 and name CB)	10.98	1.03	1.03
	assign (segid 3A4 and resid 156 and name CB)	(segid 3A4 and resid 188 and name CA)	11.88	1.35	1.35
	assign (segid 3A4 and resid 156 and name CB)	(segid 3A4 and resid 189 and name CA)	10.93	1.93	1.92
	assign (segid 3A4 and resid 156 and name CB)	(segid 3A4 and resid 189 and name CB)	11.37	2.12	2.11
10	assign (segid 3A4 and resid 156 and name CB)	(segid 3A4 and resid 190 and name CA)	7.30	1.93	1.93
	assign (segid 3A4 and resid 156 and name CB)	(segid 3A4 and resid 190 and name CB)	6.73	1.71	1.72
	assign (segid 3A4 and resid 156 and name CB)	(segid 3A4 and resid 191 and name CA)	8.27	1.21	1.21
	assign (segid 3A4 and resid 156 and name CB)	(segid 3A4 and resid 191 and name CB)	9.31	0.94	0.93
	assign (segid 3A4 and resid 156 and name CB)	(segid 3A4 and resid 192 and name CA)	10.62	1.75	1.74
	assign (segid 3A4 and resid 156 and name CB)	(segid 3A4 and resid 192 and name CB)	11.68	1.74	1.74
15	assign (segid 3A4 and resid 156 and name CB)	(segid 3A4 and resid 193 and name CA)	8.79	2.26	2.25
	assign (segid 3A4 and resid 156 and name CB)	(segid 3A4 and resid 193 and name CB)	8.05	2.42	2.42
	assign (segid 3A4 and resid 156 and name CB)	(segid 3A4 and resid 194 and name CA)	7.24	1.75	1.74
	assign (segid 3A4 and resid 156 and name CB)	(segid 3A4 and resid 194 and name CB)	6.48	1.50	1.51
	assign (segid 3A4 and resid 156 and name CB)	(segid 3A4 and resid 195 and name CA)	10.56	1.49	1.50
20	assign (segid 3A4 and resid 156 and name CB)	(segid 3A4 and resid 195 and name CB)	11.31	1.40	1.40
	assign (segid 3A4 and resid 156 and name CB)	(segid 3A4 and resid 196 and name CA)	12.25	1.99	2.00
	assign (segid 3A4 and resid 156 and name CB)	(segid 3A4 and resid 196 and name CB)	12.35	2.17	2.16
	assign (segid 3A4 and resid 156 and name CB)	(segid 3A4 and resid 197 and name CA)	11.08	2.14	2.15
	assign (segid 3A4 and resid 156 and name CB)	(segid 3A4 and resid 197 and name CB)	9.81	2.27	2.26
25	assign (segid 3A4 and resid 156 and name CB)	(segid 3A4 and resid 198 and name CA)	12.04	1.65	1.65
	assign (segid 3A4 and resid 156 and name CB)	(segid 3A4 and resid 198 and name CB)	11.53	1.47	1.47
	assign (segid 3A4 and resid 156 and name CB)	(segid 3A4 and resid 199 and name CA)	15.08	1.55	1.55
	assign (segid 3A4 and resid 156 and name CB)	(segid 3A4 and resid 199 and name CB)	15.26	1.53	1.53
	assign (segid 3A4 and resid 156 and name CB)	(segid 3A4 and resid 242 and name CA)	18.48	1.17	1.17
30	assign (segid 3A4 and resid 156 and name CB)	(segid 3A4 and resid 244 and name CA)	17.80	1.36	1.36
	assign (segid 3A4 and resid 156 and name CB)	(segid 3A4 and resid 245 and name CA)	14.57	1.43	1.43
	assign (segid 3A4 and resid 156 and name CB)	(segid 3A4 and resid 245 and name CB)	14.58	1.44	1.45
	assign (segid 3A4 and resid 156 and name CB)	(segid 3A4 and resid 246 and name CA)	13.99	1.34	1.34
	assign (segid 3A4 and resid 156 and name CB)	(segid 3A4 and resid 246 and name CB)	15.00	1.33	1.33
35	assign (segid 3A4 and resid 156 and name CB)	(segid 3A4 and resid 247 and name CA)	15.04	1.51	1.51
	assign (segid 3A4 and resid 156 and name CB)	(segid 3A4 and resid 247 and name CB)	16.38	1.55	1.54
	assign (segid 3A4 and resid 156 and name CB)	(segid 3A4 and resid 248 and name CA)	12.92	1.66	1.66
	assign (segid 3A4 and resid 156 and name CB)	(segid 3A4 and resid 248 and name CB)	13.06	1.76	1.75
40	assign (segid 3A4 and resid 156 and name CB)	(segid 3A4 and resid 249 and name CA)	9.91	1.48	1.48
	assign (segid 3A4 and resid 156 and name CB)	(segid 3A4 and resid 250 and name CA)	11.55	1.49	1.50
	assign (segid 3A4 and resid 156 and name CB)	(segid 3A4 and resid 250 and name CB)	12.90	1.51	1.51
	assign (segid 3A4 and resid 156 and name CB)	(segid 3A4 and resid 251 and name CA)	12.54	1.55	1.55
	assign (segid 3A4 and resid 156 and name CB)	(segid 3A4 and resid 251 and name CB)	13.43	1.57	1.56
45	assign (segid 3A4 and resid 156 and name CB)	(segid 3A4 and resid 252 and name CA)	9.40	1.55	1.54
	assign (segid 3A4 and resid 156 and name CB)	(segid 3A4 and resid 252 and name CB)	8.54	1.54	1.54
	assign (segid 3A4 and resid 156 and name CB)	(segid 3A4 and resid 253 and name CA)	8.17	1.64	1.64
	assign (segid 3A4 and resid 156 and name CB)	(segid 3A4 and resid 254 and name CA)	11.66	1.78	1.78
	assign (segid 3A4 and resid 156 and name CB)	(segid 3A4 and resid 255 and name CA)	12.54	1.70	1.70
	assign (segid 3A4 and resid 156 and name CB)	(segid 3A4 and resid 256 and name CA)	10.62	1.67	1.68
50	assign (segid 3A4 and resid 156 and name CB)	(segid 3A4 and resid 257 and name CA)	10.85	1.52	1.53
	assign (segid 3A4 and resid 156 and name CB)	(segid 3A4 and resid 258 and name CA)	14.20	1.61	1.61
	assign (segid 3A4 and resid 156 and name CB)	(segid 3A4 and resid 258 and name CB)	14.66	1.69	1.70
	assign (segid 3A4 and resid 156 and name CB)	(segid 3A4 and resid 259 and name CA)	15.75	1.45	1.45
	assign (segid 3A4 and resid 156 and name CB)	(segid 3A4 and resid 259 and name CB)	15.65	1.51	1.50
55	assign (segid 3A4 and resid 156 and name CB)	(segid 3A4 and resid 260 and name CA)	14.74	1.31	1.30
	assign (segid 3A4 and resid 156 and name CB)	(segid 3A4 and resid 260 and name CB)	13.49	1.29	1.29
	assign (segid 3A4 and resid 156 and name CB)	(segid 3A4 and resid 261 and name CA)	16.15	1.54	1.54
	assign (segid 3A4 and resid 156 and name N)	(segid 3A4 and resid 156 and name C)	2.48	0.04	0.03
60	assign (segid 3A4 and resid 156 and name N)	(segid 3A4 and resid 156 and name CB)	1.46	0.01	0.01
	assign (segid 3A4 and resid 156 and name N)	(segid 3A4 and resid 156 and name O)	2.45	0.04	0.03
	assign (segid 3A4 and resid 156 and name N)	(segid 3A4 and resid 157 and name C)	3.50	0.04	0.03
	assign (segid 3A4 and resid 156 and name N)	(segid 3A4 and resid 157 and name CA)	4.75	0.10	0.11
	assign (segid 3A4 and resid 156 and name N)	(segid 3A4 and resid 157 and name CB)	4.23	0.08	0.09
65	assign (segid 3A4 and resid 156 and name N)	(segid 3A4 and resid 157 and name N)	5.00	0.19	0.18
	assign (segid 3A4 and resid 156 and name N)	(segid 3A4 and resid 157 and name O)	2.84	0.08	0.07
	assign (segid 3A4 and resid 156 and name N)	(segid 3A4 and resid 158 and name C)	5.83	0.10	0.09
	assign (segid 3A4 and resid 156 and name N)	(segid 3A4 and resid 158 and name CA)	5.72	0.15	0.15
	assign (segid 3A4 and resid 156 and name N)	(segid 3A4 and resid 158 and name CB)	5.42	0.20	0.19
	assign (segid 3A4 and resid 156 and name N)	(segid 3A4 and resid 158 and name N)	5.52	0.30	0.31
70	assign (segid 3A4 and resid 156 and name N)	(segid 3A4 and resid 158 and name O)	4.38	0.17	0.18
	assign (segid 3A4 and resid 156 and name N)	(segid 3A4 and resid 159 and name C)	6.90	0.15	0.15
	assign (segid 3A4 and resid 156 and name N)	(segid 3A4 and resid 159 and name CA)	6.53	0.34	0.33
	assign (segid 3A4 and resid 156 and name N)	(segid 3A4 and resid 159 and name CB)	5.74	0.16	0.16
	assign (segid 3A4 and resid 156 and name N)	(segid 3A4 and resid 159 and name N)	5.28	0.18	0.17
75	assign (segid 3A4 and resid 156 and name N)	(segid 3A4 and resid 159 and name O)	4.93	0.15	0.16
	assign (segid 3A4 and resid 156 and name N)	(segid 3A4 and resid 160 and name CA)	7.26	0.63	0.63
	assign (segid 3A4 and resid 156 and name N)	(segid 3A4 and resid 160 and name CB)	7.04	0.79	0.78
	assign (segid 3A4 and resid 156 and name N)	(segid 3A4 and resid 160 and name N)	6.15	0.50	0.50
80	assign (segid 3A4 and resid 156 and name O)	(segid 3A4 and resid 156 and name CB)	3.35	0.05	0.05
	assign (segid 3A4 and resid 156 and name O)	(segid 3A4 and resid 157 and name C)	3.07	0.09	0.09
	assign (segid 3A4 and resid 156 and name O)	(segid 3A4 and resid 157 and name CA)	2.81	0.04	0.05
	assign (segid 3A4 and resid 156 and name O)	(segid 3A4 and resid 157 and name CB)	4.29	0.06	0.06

	assign (segid 3A4 and resid 156 and name O)	(segid 3A4 and resid 157 and name N)	2.27	0.02	0.01
	assign (segid 3A4 and resid 156 and name O)	(segid 3A4 and resid 157 and name O)	3.52	0.06	0.07
	assign (segid 3A4 and resid 156 and name O)	(segid 3A4 and resid 158 and name C)	4.25	0.28	0.29
	assign (segid 3A4 and resid 156 and name O)	(segid 3A4 and resid 158 and name CA)	4.50	0.24	0.24
5	assign (segid 3A4 and resid 156 and name O)	(segid 3A4 and resid 158 and name CB)	5.47	0.33	0.33
	assign (segid 3A4 and resid 156 and name O)	(segid 3A4 and resid 158 and name N)	3.54	0.21	0.20
	assign (segid 3A4 and resid 156 and name O)	(segid 3A4 and resid 158 and name O)	5.13	0.20	0.21
	assign (segid 3A4 and resid 156 and name O)	(segid 3A4 and resid 159 and name C)	4.06	0.23	0.23
	assign (segid 3A4 and resid 156 and name O)	(segid 3A4 and resid 159 and name CA)	3.97	0.47	0.48
	assign (segid 3A4 and resid 156 and name O)	(segid 3A4 and resid 159 and name CB)	3.92	0.73	0.73
10	assign (segid 3A4 and resid 156 and name O)	(segid 3A4 and resid 159 and name N)	3.49	0.43	0.43
	assign (segid 3A4 and resid 156 and name O)	(segid 3A4 and resid 159 and name O)	5.15	0.12	0.11
	assign (segid 3A4 and resid 156 and name O)	(segid 3A4 and resid 160 and name C)	5.17	0.51	0.52
	assign (segid 3A4 and resid 156 and name O)	(segid 3A4 and resid 160 and name CA)	4.20	0.15	0.16
	assign (segid 3A4 and resid 156 and name O)	(segid 3A4 and resid 160 and name CB)	4.00	0.21	0.22
15	assign (segid 3A4 and resid 156 and name O)	(segid 3A4 and resid 160 and name N)	3.36	0.19	0.19
	assign (segid 3A4 and resid 156 and name O)	(segid 3A4 and resid 160 and name O)	6.29	0.50	0.50
	assign (segid 3A4 and resid 156 and name O)	(segid 3A4 and resid 161 and name C)	7.14	1.01	1.00
	assign (segid 3A4 and resid 156 and name O)	(segid 3A4 and resid 161 and name CA)	6.32	0.99	0.99
	assign (segid 3A4 and resid 156 and name O)	(segid 3A4 and resid 161 and name CB)	6.49	1.18	1.18
20	assign (segid 3A4 and resid 156 and name O)	(segid 3A4 and resid 161 and name N)	5.05	0.81	0.82
	assign (segid 3A4 and resid 156 and name O)	(segid 3A4 and resid 161 and name O)	2.50	0.02	0.03
	assign (segid 3A4 and resid 157 and name C)	(segid 3A4 and resid 157 and name O)	1.23	0.01	0.00
	assign (segid 3A4 and resid 157 and name C)	(segid 3A4 and resid 158 and name C)	3.03	0.10	0.10
	assign (segid 3A4 and resid 157 and name C)	(segid 3A4 and resid 158 and name CA)	2.43	0.01	0.01
25	assign (segid 3A4 and resid 157 and name C)	(segid 3A4 and resid 158 and name CB)	3.69	0.04	0.03
	assign (segid 3A4 and resid 157 and name C)	(segid 3A4 and resid 158 and name N)	1.33	0.01	0.00
	assign (segid 3A4 and resid 157 and name C)	(segid 3A4 and resid 158 and name O)	3.84	0.12	0.13
	assign (segid 3A4 and resid 157 and name C)	(segid 3A4 and resid 159 and name C)	4.65	0.20	0.20
	assign (segid 3A4 and resid 157 and name C)	(segid 3A4 and resid 159 and name CA)	4.51	0.19	0.20
30	assign (segid 3A4 and resid 157 and name C)	(segid 3A4 and resid 159 and name CB)	5.31	0.30	0.30
	assign (segid 3A4 and resid 157 and name C)	(segid 3A4 and resid 159 and name N)	3.33	0.18	0.17
	assign (segid 3A4 and resid 157 and name C)	(segid 3A4 and resid 159 and name O)	5.67	0.10	0.11
	assign (segid 3A4 and resid 157 and name C)	(segid 3A4 and resid 160 and name C)	5.15	0.22	0.22
	assign (segid 3A4 and resid 157 and name C)	(segid 3A4 and resid 160 and name CA)	4.85	0.41	0.40
35	assign (segid 3A4 and resid 157 and name C)	(segid 3A4 and resid 160 and name CB)	4.79	0.60	0.61
	assign (segid 3A4 and resid 157 and name C)	(segid 3A4 and resid 160 and name N)	4.04	0.40	0.41
	assign (segid 3A4 and resid 157 and name C)	(segid 3A4 and resid 160 and name O)	6.32	0.19	0.20
	assign (segid 3A4 and resid 157 and name C)	(segid 3A4 and resid 161 and name C)	6.02	0.59	0.60
	assign (segid 3A4 and resid 157 and name C)	(segid 3A4 and resid 161 and name CA)	5.26	0.31	0.31
40	assign (segid 3A4 and resid 157 and name C)	(segid 3A4 and resid 161 and name CB)	4.98	0.37	0.36
	assign (segid 3A4 and resid 157 and name C)	(segid 3A4 and resid 161 and name N)	4.43	0.21	0.20
	assign (segid 3A4 and resid 157 and name C)	(segid 3A4 and resid 161 and name O)	6.96	0.92	0.92
	assign (segid 3A4 and resid 157 and name CA)	(segid 3A4 and resid 157 and name CB)	1.52	0.01	0.01
	assign (segid 3A4 and resid 157 and name CA)	(segid 3A4 and resid 157 and name N)	1.54	0.02	0.02
45	assign (segid 3A4 and resid 157 and name CA)	(segid 3A4 and resid 157 and name O)	2.38	0.03	0.02
	assign (segid 3A4 and resid 157 and name CA)	(segid 3A4 and resid 158 and name C)	4.42	0.07	0.08
	assign (segid 3A4 and resid 157 and name CA)	(segid 3A4 and resid 158 and name CA)	3.80	0.01	0.01
	assign (segid 3A4 and resid 157 and name CA)	(segid 3A4 and resid 158 and name CB)	4.85	0.04	0.03
	assign (segid 3A4 and resid 157 and name CA)	(segid 3A4 and resid 158 and name N)	2.43	0.01	0.01
50	assign (segid 3A4 and resid 157 and name CA)	(segid 3A4 and resid 158 and name O)	5.30	0.12	0.12
	assign (segid 3A4 and resid 157 and name CA)	(segid 3A4 and resid 159 and name C)	5.60	0.17	0.16
	assign (segid 3A4 and resid 157 and name CA)	(segid 3A4 and resid 159 and name CA)	5.51	0.20	0.19
	assign (segid 3A4 and resid 157 and name CA)	(segid 3A4 and resid 159 and name CB)	5.99	0.34	0.34
	assign (segid 3A4 and resid 157 and name CA)	(segid 3A4 and resid 159 and name N)	4.42	0.15	0.15
55	assign (segid 3A4 and resid 157 and name CA)	(segid 3A4 and resid 159 and name O)	6.67	0.10	0.10
	assign (segid 3A4 and resid 157 and name CA)	(segid 3A4 and resid 160 and name C)	5.95	0.19	0.20
	assign (segid 3A4 and resid 157 and name CA)	(segid 3A4 and resid 160 and name CA)	5.45	0.32	0.32
	assign (segid 3A4 and resid 157 and name CA)	(segid 3A4 and resid 160 and name CB)	5.01	0.52	0.52
	assign (segid 3A4 and resid 157 and name CA)	(segid 3A4 and resid 160 and name N)	4.80	0.32	0.32
60	assign (segid 3A4 and resid 157 and name CA)	(segid 3A4 and resid 160 and name O)	7.09	0.21	0.22
	assign (segid 3A4 and resid 157 and name CA)	(segid 3A4 and resid 161 and name CA)	6.30	0.55	0.55
	assign (segid 3A4 and resid 157 and name CA)	(segid 3A4 and resid 161 and name CB)	5.97	0.63	0.64
	assign (segid 3A4 and resid 157 and name CA)	(segid 3A4 and resid 161 and name N)	5.40	0.33	0.34
	assign (segid 3A4 and resid 157 and name CA)	(segid 3A4 and resid 187 and name CA)	10.35	1.49	1.50
65	assign (segid 3A4 and resid 157 and name CA)	(segid 3A4 and resid 187 and name CB)	10.71	1.53	1.52
	assign (segid 3A4 and resid 157 and name CA)	(segid 3A4 and resid 188 and name CA)	12.84	1.53	1.54
	assign (segid 3A4 and resid 157 and name CA)	(segid 3A4 and resid 189 and name CA)	12.70	1.67	1.67
	assign (segid 3A4 and resid 157 and name CA)	(segid 3A4 and resid 189 and name CB)	13.09	1.82	1.82
	assign (segid 3A4 and resid 157 and name CA)	(segid 3A4 and resid 190 and name CA)	9.16	1.76	1.76
70	assign (segid 3A4 and resid 157 and name CA)	(segid 3A4 and resid 190 and name CB)	8.04	1.72	1.73
	assign (segid 3A4 and resid 157 and name CA)	(segid 3A4 and resid 191 and name CA)	9.90	1.57	1.58
	assign (segid 3A4 and resid 157 and name CA)	(segid 3A4 and resid 191 and name CB)	10.56	1.37	1.37
	assign (segid 3A4 and resid 157 and name CA)	(segid 3A4 and resid 192 and name CA)	13.02	1.69	1.68
	assign (segid 3A4 and resid 157 and name CA)	(segid 3A4 and resid 192 and name CB)	14.03	1.55	1.56
75	assign (segid 3A4 and resid 157 and name CA)	(segid 3A4 and resid 193 and name CA)	11.89	1.90	1.90
	assign (segid 3A4 and resid 157 and name CA)	(segid 3A4 and resid 193 and name CB)	11.19	1.92	1.92
	assign (segid 3A4 and resid 157 and name CA)	(segid 3A4 and resid 194 and name CA)	10.08	2.00	2.00
	assign (segid 3A4 and resid 157 and name CA)	(segid 3A4 and resid 194 and name CB)	8.93	2.02	2.01
	assign (segid 3A4 and resid 157 and name CA)	(segid 3A4 and resid 195 and name CA)	13.18	1.85	1.85
80	assign (segid 3A4 and resid 157 and name CA)	(segid 3A4 and resid 195 and name CB)	13.73	1.76	1.77
	assign (segid 3A4 and resid 157 and name CA)	(segid 3A4 and resid 196 and name CA)	15.42	1.96	1.95
	assign (segid 3A4 and resid 157 and name CA)	(segid 3A4 and resid 196 and name CB)	15.60	1.96	1.96

	assign (segid 3A4 and resid 157 and name CA) (segid 3A4 and resid 197 and name CA)	14.30	2.19	2.19
	assign (segid 3A4 and resid 157 and name CA) (segid 3A4 and resid 197 and name CB)	13.01	2.30	2.30
	assign (segid 3A4 and resid 157 and name CA) (segid 3A4 and resid 198 and name CA)	14.81	2.08	2.07
	assign (segid 3A4 and resid 157 and name CA) (segid 3A4 and resid 198 and name CB)	14.08	2.00	2.00
5	assign (segid 3A4 and resid 157 and name CA) (segid 3A4 and resid 246 and name CA)	15.29	1.26	1.26
	assign (segid 3A4 and resid 157 and name CA) (segid 3A4 and resid 246 and name CB)	16.17	1.11	1.12
	assign (segid 3A4 and resid 157 and name CA) (segid 3A4 and resid 247 and name CA)	16.00	1.47	1.47
	assign (segid 3A4 and resid 157 and name CA) (segid 3A4 and resid 247 and name CB)	14.27	1.84	1.84
	assign (segid 3A4 and resid 157 and name CA) (segid 3A4 and resid 248 and name CA)	14.73	1.95	1.94
	assign (segid 3A4 and resid 157 and name CA) (segid 3A4 and resid 248 and name CB)	11.08	1.65	1.65
10	assign (segid 3A4 and resid 157 and name CA) (segid 3A4 and resid 249 and name CA)	11.72	1.44	1.44
	assign (segid 3A4 and resid 157 and name CA) (segid 3A4 and resid 250 and name CA)	13.02	1.38	1.38
	assign (segid 3A4 and resid 157 and name CA) (segid 3A4 and resid 250 and name CB)	12.69	1.71	1.72
	assign (segid 3A4 and resid 157 and name CA) (segid 3A4 and resid 251 and name CA)	13.83	1.77	1.78
	assign (segid 3A4 and resid 157 and name CA) (segid 3A4 and resid 251 and name CB)	9.69	1.90	1.89
15	assign (segid 3A4 and resid 157 and name CA) (segid 3A4 and resid 252 and name CA)	9.28	1.95	1.95
	assign (segid 3A4 and resid 157 and name CA) (segid 3A4 and resid 252 and name CB)	7.44	1.57	1.58
	assign (segid 3A4 and resid 157 and name CA) (segid 3A4 and resid 253 and name CA)	10.46	1.32	1.31
	assign (segid 3A4 and resid 157 and name CA) (segid 3A4 and resid 253 and name CB)	11.55	1.65	1.65
	assign (segid 3A4 and resid 157 and name CA) (segid 3A4 and resid 254 and name CA)	9.30	1.92	1.92
	assign (segid 3A4 and resid 157 and name CA) (segid 3A4 and resid 254 and name CB)	8.55	1.52	1.53
20	assign (segid 3A4 and resid 157 and name CA) (segid 3A4 and resid 255 and name CA)	11.90	1.26	1.26
	assign (segid 3A4 and resid 157 and name CA) (segid 3A4 and resid 255 and name CB)	12.51	1.20	1.19
	assign (segid 3A4 and resid 157 and name CA) (segid 3A4 and resid 256 and name CA)	13.80	1.48	1.48
	assign (segid 3A4 and resid 157 and name CA) (segid 3A4 and resid 256 and name CB)	13.96	1.64	1.64
25	assign (segid 3A4 and resid 157 and name CA) (segid 3A4 and resid 257 and name CA)	12.62	1.64	1.63
	assign (segid 3A4 and resid 157 and name CA) (segid 3A4 and resid 257 and name CB)	11.36	1.75	1.76
	assign (segid 3A4 and resid 157 and name CA) (segid 3A4 and resid 258 and name CA)	13.49	1.29	1.30
	assign (segid 3A4 and resid 157 and name CA) (segid 3A4 and resid 258 and name CB)	16.62	1.29	1.29
	assign (segid 3A4 and resid 157 and name CA) (segid 3A4 and resid 259 and name CA)	16.09	0.90	0.90
	assign (segid 3A4 and resid 157 and name CA) (segid 3A4 and resid 259 and name CB)	15.45	0.92	0.91
30	assign (segid 3A4 and resid 157 and name CA) (segid 3A4 and resid 260 and name CA)	15.68	0.98	0.97
	assign (segid 3A4 and resid 157 and name CA) (segid 3A4 and resid 260 and name CB)	15.64	0.81	0.80
	assign (segid 3A4 and resid 157 and name CA) (segid 3A4 and resid 261 and name CA)	18.42	0.97	0.98
	assign (segid 3A4 and resid 157 and name CA) (segid 3A4 and resid 261 and name CB)	15.97	1.29	1.30
35	assign (segid 3A4 and resid 157 and name CA) (segid 3A4 and resid 262 and name CA)	15.62	1.79	1.78
	assign (segid 3A4 and resid 157 and name CA) (segid 3A4 and resid 262 and name CB)	13.11	2.50	2.50
	assign (segid 3A4 and resid 157 and name CA) (segid 3A4 and resid 263 and name CA)	14.40	1.74	1.75
	assign (segid 3A4 and resid 157 and name CA) (segid 3A4 and resid 263 and name CB)	14.26	1.24	1.24
40	assign (segid 3A4 and resid 157 and name CA) (segid 3A4 and resid 264 and name CA)	15.81	0.83	0.84
	assign (segid 3A4 and resid 157 and name CA) (segid 3A4 and resid 264 and name CB)	14.84	1.26	1.26
	assign (segid 3A4 and resid 157 and name CA) (segid 3A4 and resid 265 and name CA)	16.96	0.79	0.79
	assign (segid 3A4 and resid 157 and name CA) (segid 3A4 and resid 265 and name CB)	5.44	0.08	0.08
	assign (segid 3A4 and resid 157 and name CB) (segid 3A4 and resid 158 and name CA)	4.48	0.05	0.04
45	assign (segid 3A4 and resid 157 and name CB) (segid 3A4 and resid 158 and name CB)	5.32	0.10	0.10
	assign (segid 3A4 and resid 157 and name CB) (segid 3A4 and resid 158 and name N)	3.17	0.06	0.05
	assign (segid 3A4 and resid 157 and name CB) (segid 3A4 and resid 158 and name O)	6.28	0.12	0.12
	assign (segid 3A4 and resid 157 and name CB) (segid 3A4 and resid 159 and name C)	7.01	0.18	0.17
	assign (segid 3A4 and resid 157 and name CB) (segid 3A4 and resid 159 and name CA)	6.86	0.17	0.18
	assign (segid 3A4 and resid 157 and name CB) (segid 3A4 and resid 159 and name CB)	7.41	0.30	0.29
50	assign (segid 3A4 and resid 157 and name CB) (segid 3A4 and resid 159 and name N)	5.66	0.14	0.14
	assign (segid 3A4 and resid 157 and name CB) (segid 3A4 and resid 160 and name C)	7.14	0.25	0.24
	assign (segid 3A4 and resid 157 and name CB) (segid 3A4 and resid 160 and name CA)	6.79	0.40	0.40
	assign (segid 3A4 and resid 157 and name CB) (segid 3A4 and resid 160 and name CB)	6.26	0.63	0.63
	assign (segid 3A4 and resid 157 and name CB) (segid 3A4 and resid 160 and name N)	6.22	0.36	0.35
55	assign (segid 3A4 and resid 157 and name CB) (segid 3A4 and resid 161 and name CA)	7.14	0.42	0.42
	assign (segid 3A4 and resid 157 and name CB) (segid 3A4 and resid 161 and name CB)	6.55	0.49	0.49
	assign (segid 3A4 and resid 157 and name CB) (segid 3A4 and resid 161 and name N)	6.45	0.25	0.25
	assign (segid 3A4 and resid 157 and name CB) (segid 3A4 and resid 161 and name O)	11.51	1.64	1.64
60	assign (segid 3A4 and resid 157 and name CB) (segid 3A4 and resid 162 and name CA)	11.88	1.71	1.71
	assign (segid 3A4 and resid 157 and name CB) (segid 3A4 and resid 162 and name CB)	13.93	1.56	1.56
	assign (segid 3A4 and resid 157 and name CB) (segid 3A4 and resid 163 and name CA)	13.68	1.62	1.62
	assign (segid 3A4 and resid 157 and name CB) (segid 3A4 and resid 163 and name CB)	14.06	1.82	1.81
	assign (segid 3A4 and resid 157 and name CB) (segid 3A4 and resid 164 and name CA)	10.14	1.64	1.64
	assign (segid 3A4 and resid 157 and name CB) (segid 3A4 and resid 164 and name CB)	9.09	1.63	1.64
65	assign (segid 3A4 and resid 157 and name CB) (segid 3A4 and resid 165 and name CA)	10.82	1.49	1.49
	assign (segid 3A4 and resid 157 and name CB) (segid 3A4 and resid 165 and name CB)	11.52	1.33	1.33
	assign (segid 3A4 and resid 157 and name CB) (segid 3A4 and resid 166 and name CA)	13.79	1.57	1.56
	assign (segid 3A4 and resid 157 and name CB) (segid 3A4 and resid 166 and name CB)	14.84	1.43	1.43
	assign (segid 3A4 and resid 157 and name CB) (segid 3A4 and resid 167 and name CA)	12.50	1.72	1.72
70	assign (segid 3A4 and resid 157 and name CB) (segid 3A4 and resid 167 and name CB)	11.82	1.72	1.73
	assign (segid 3A4 and resid 157 and name CB) (segid 3A4 and resid 168 and name CA)	10.51	1.97	1.97
	assign (segid 3A4 and resid 157 and name CB) (segid 3A4 and resid 168 and name CB)	9.40	2.04	2.03
	assign (segid 3A4 and resid 157 and name CB) (segid 3A4 and resid 169 and name CA)	13.63	1.88	1.89
	assign (segid 3A4 and resid 157 and name CB) (segid 3A4 and resid 169 and name CB)	14.27	1.79	1.79
75	assign (segid 3A4 and resid 157 and name CB) (segid 3A4 and resid 170 and name CA)	15.80	1.89	1.88
	assign (segid 3A4 and resid 157 and name CB) (segid 3A4 and resid 170 and name CB)	16.03	1.84	1.84
	assign (segid 3A4 and resid 157 and name CB) (segid 3A4 and resid 171 and name CA)	14.41	2.15	2.15
	assign (segid 3A4 and resid 157 and name CB) (segid 3A4 and resid 171 and name CB)	13.10	2.25	2.25
80	assign (segid 3A4 and resid 157 and name CB) (segid 3A4 and resid 172 and name CA)	14.82	2.21	2.21
	assign (segid 3A4 and resid 157 and name CB) (segid 3A4 and resid 172 and name CB)	14.13	2.18	2.18
	assign (segid 3A4 and resid 157 and name CB) (segid 3A4 and resid 173 and name CA)	15.56	1.53	1.53
	assign (segid 3A4 and resid 157 and name CB) (segid 3A4 and resid 173 and name CB)	16.52	1.39	1.38

	assign (segid 3A4 and resid 157 and name CB)	(segid 3A4 and resid 248 and name CA)	14.10	2.17	2.18
	assign (segid 3A4 and resid 157 and name CB)	(segid 3A4 and resid 248 and name CB)	14.56	2.23	2.24
	assign (segid 3A4 and resid 157 and name CB)	(segid 3A4 and resid 249 and name CA)	11.13	1.92	1.92
	assign (segid 3A4 and resid 157 and name CB)	(segid 3A4 and resid 250 and name CA)	11.71	1.86	1.86
5	assign (segid 3A4 and resid 157 and name CB)	(segid 3A4 and resid 250 and name CB)	13.05	1.80	1.81
	assign (segid 3A4 and resid 157 and name CB)	(segid 3A4 and resid 251 and name CA)	12.30	2.22	2.22
	assign (segid 3A4 and resid 157 and name CB)	(segid 3A4 and resid 251 and name CB)	13.40	2.26	2.26
	assign (segid 3A4 and resid 157 and name CB)	(segid 3A4 and resid 252 and name CA)	9.15	2.35	2.35
	assign (segid 3A4 and resid 157 and name CB)	(segid 3A4 and resid 252 and name CB)	8.82	2.34	2.34
	assign (segid 3A4 and resid 157 and name CB)	(segid 3A4 and resid 253 and name CA)	7.16	2.04	2.05
10	assign (segid 3A4 and resid 157 and name CB)	(segid 3A4 and resid 254 and name CA)	10.12	1.85	1.85
	assign (segid 3A4 and resid 157 and name CB)	(segid 3A4 and resid 255 and name CA)	10.88	2.22	2.22
	assign (segid 3A4 and resid 157 and name CB)	(segid 3A4 and resid 256 and name CA)	8.44	2.39	2.39
	assign (segid 3A4 and resid 157 and name CB)	(segid 3A4 and resid 257 and name CA)	7.97	1.89	1.88
	assign (segid 3A4 and resid 157 and name CB)	(segid 3A4 and resid 258 and name CA)	11.37	1.67	1.67
15	assign (segid 3A4 and resid 157 and name CB)	(segid 3A4 and resid 258 and name CB)	12.02	1.66	1.66
	assign (segid 3A4 and resid 157 and name CB)	(segid 3A4 and resid 259 and name CA)	13.02	1.92	1.91
	assign (segid 3A4 and resid 157 and name CB)	(segid 3A4 and resid 259 and name CB)	13.11	2.08	2.08
	assign (segid 3A4 and resid 157 and name CB)	(segid 3A4 and resid 260 and name CA)	11.79	1.93	1.94
	assign (segid 3A4 and resid 157 and name CB)	(segid 3A4 and resid 260 and name CB)	10.54	2.02	2.03
20	assign (segid 3A4 and resid 157 and name CB)	(segid 3A4 and resid 261 and name CA)	12.90	1.54	1.54
	assign (segid 3A4 and resid 157 and name CB)	(segid 3A4 and resid 318 and name CB)	15.87	1.07	1.08
	assign (segid 3A4 and resid 157 and name CB)	(segid 3A4 and resid 318 and name CB)	15.15	1.18	1.18
	assign (segid 3A4 and resid 157 and name CB)	(segid 3A4 and resid 319 and name CA)	15.66	1.10	1.09
25	assign (segid 3A4 and resid 157 and name CB)	(segid 3A4 and resid 319 and name CB)	15.58	1.00	1.00
	assign (segid 3A4 and resid 157 and name CB)	(segid 3A4 and resid 426 and name CA)	18.35	1.03	1.03
	assign (segid 3A4 and resid 157 and name CB)	(segid 3A4 and resid 427 and name CA)	16.05	1.28	1.28
	assign (segid 3A4 and resid 157 and name CB)	(segid 3A4 and resid 431 and name CA)	13.58	2.35	2.35
	assign (segid 3A4 and resid 157 and name CB)	(segid 3A4 and resid 433 and name CA)	14.38	1.75	1.75
	assign (segid 3A4 and resid 157 and name CB)	(segid 3A4 and resid 434 and name CA)	13.99	1.30	1.30
30	assign (segid 3A4 and resid 157 and name CB)	(segid 3A4 and resid 435 and name CA)	15.48	0.97	0.96
	assign (segid 3A4 and resid 157 and name CB)	(segid 3A4 and resid 436 and name CA)	14.55	1.20	1.19
	assign (segid 3A4 and resid 157 and name CB)	(segid 3A4 and resid 437 and name CA)	16.51	0.76	0.76
	assign (segid 3A4 and resid 157 and name N)	(segid 3A4 and resid 157 and name C)	2.46	0.03	0.03
35	assign (segid 3A4 and resid 157 and name N)	(segid 3A4 and resid 157 and name CB)	1.46	0.01	0.00
	assign (segid 3A4 and resid 157 and name N)	(segid 3A4 and resid 157 and name O)	2.46	0.04	0.05
	assign (segid 3A4 and resid 157 and name N)	(segid 3A4 and resid 157 and name O)	3.48	0.03	0.03
	assign (segid 3A4 and resid 157 and name N)	(segid 3A4 and resid 158 and name C)	4.73	0.06	0.06
	assign (segid 3A4 and resid 157 and name N)	(segid 3A4 and resid 158 and name CA)	4.23	0.07	0.06
	assign (segid 3A4 and resid 157 and name N)	(segid 3A4 and resid 158 and name CB)	4.99	0.09	0.09
40	assign (segid 3A4 and resid 157 and name N)	(segid 3A4 and resid 158 and name N)	2.82	0.06	0.07
	assign (segid 3A4 and resid 157 and name N)	(segid 3A4 and resid 158 and name O)	5.78	0.09	0.09
	assign (segid 3A4 and resid 157 and name N)	(segid 3A4 and resid 159 and name C)	5.71	0.06	0.06
	assign (segid 3A4 and resid 157 and name N)	(segid 3A4 and resid 159 and name CA)	5.39	0.15	0.16
	assign (segid 3A4 and resid 157 and name N)	(segid 3A4 and resid 159 and name CB)	5.52	0.32	0.33
45	assign (segid 3A4 and resid 157 and name N)	(segid 3A4 and resid 159 and name N)	4.37	0.13	0.13
	assign (segid 3A4 and resid 157 and name N)	(segid 3A4 and resid 159 and name O)	6.87	0.11	0.10
	assign (segid 3A4 and resid 157 and name N)	(segid 3A4 and resid 160 and name C)	6.61	0.32	0.31
	assign (segid 3A4 and resid 157 and name N)	(segid 3A4 and resid 160 and name CA)	5.85	0.11	0.11
	assign (segid 3A4 and resid 157 and name N)	(segid 3A4 and resid 160 and name CB)	5.44	0.18	0.18
50	assign (segid 3A4 and resid 157 and name N)	(segid 3A4 and resid 160 and name N)	5.00	0.10	0.11
	assign (segid 3A4 and resid 157 and name N)	(segid 3A4 and resid 161 and name N)	6.19	0.52	0.53
	assign (segid 3A4 and resid 157 and name O)	(segid 3A4 and resid 157 and name CB)	3.28	0.05	0.06
	assign (segid 3A4 and resid 157 and name O)	(segid 3A4 and resid 158 and name C)	3.00	0.16	0.17
55	assign (segid 3A4 and resid 157 and name O)	(segid 3A4 and resid 158 and name CA)	2.77	0.03	0.02
	assign (segid 3A4 and resid 157 and name O)	(segid 3A4 and resid 158 and name CB)	4.23	0.05	0.04
	assign (segid 3A4 and resid 157 and name O)	(segid 3A4 and resid 158 and name N)	2.24	0.00	0.01
	assign (segid 3A4 and resid 157 and name O)	(segid 3A4 and resid 158 and name O)	3.44	0.20	0.21
	assign (segid 3A4 and resid 157 and name O)	(segid 3A4 and resid 159 and name C)	4.24	0.36	0.37
	assign (segid 3A4 and resid 157 and name O)	(segid 3A4 and resid 159 and name CA)	4.46	0.30	0.30
60	assign (segid 3A4 and resid 157 and name O)	(segid 3A4 and resid 159 and name CB)	5.46	0.38	0.39
	assign (segid 3A4 and resid 157 and name O)	(segid 3A4 and resid 159 and name N)	3.49	0.24	0.25
	assign (segid 3A4 and resid 157 and name O)	(segid 3A4 and resid 159 and name O)	5.12	0.21	0.20
	assign (segid 3A4 and resid 157 and name O)	(segid 3A4 and resid 160 and name C)	4.20	0.45	0.46
	assign (segid 3A4 and resid 157 and name O)	(segid 3A4 and resid 160 and name CA)	4.13	0.68	0.68
65	assign (segid 3A4 and resid 157 and name O)	(segid 3A4 and resid 160 and name CB)	4.16	0.93	0.92
	assign (segid 3A4 and resid 157 and name O)	(segid 3A4 and resid 160 and name N)	3.57	0.66	0.65
	assign (segid 3A4 and resid 157 and name O)	(segid 3A4 and resid 160 and name O)	5.32	0.38	0.38
	assign (segid 3A4 and resid 157 and name O)	(segid 3A4 and resid 161 and name C)	4.99	0.57	0.57
	assign (segid 3A4 and resid 157 and name O)	(segid 3A4 and resid 161 and name CA)	4.20	0.30	0.29
70	assign (segid 3A4 and resid 157 and name O)	(segid 3A4 and resid 161 and name CB)	4.00	0.37	0.36
	assign (segid 3A4 and resid 157 and name O)	(segid 3A4 and resid 161 and name N)	3.42	0.37	0.37
	assign (segid 3A4 and resid 157 and name O)	(segid 3A4 and resid 161 and name O)	5.89	0.94	0.93
	assign (segid 3A4 and resid 158 and name C)	(segid 3A4 and resid 158 and name CB)	2.49	0.02	0.02
75	assign (segid 3A4 and resid 158 and name C)	(segid 3A4 and resid 158 and name O)	1.23	0.00	0.01
	assign (segid 3A4 and resid 158 and name C)	(segid 3A4 and resid 159 and name C)	3.05	0.06	0.07
	assign (segid 3A4 and resid 158 and name C)	(segid 3A4 and resid 159 and name CA)	2.43	0.02	0.01
	assign (segid 3A4 and resid 158 and name C)	(segid 3A4 and resid 159 and name CB)	3.71	0.02	0.03
	assign (segid 3A4 and resid 158 and name C)	(segid 3A4 and resid 159 and name N)	1.33	0.01	0.01
	assign (segid 3A4 and resid 158 and name C)	(segid 3A4 and resid 159 and name O)	3.87	0.13	0.13
80	assign (segid 3A4 and resid 158 and name C)	(segid 3A4 and resid 160 and name C)	4.71	0.20	0.21
	assign (segid 3A4 and resid 158 and name C)	(segid 3A4 and resid 160 and name CA)	4.58	0.22	0.22
	assign (segid 3A4 and resid 158 and name C)	(segid 3A4 and resid 160 and name CB)	5.39	0.29	0.29

assign (segid 3A4 and resid 158 and name C) (segid 3A4 and resid 160 and name N) 3.37 0.21 0.22
 assign (segid 3A4 and resid 158 and name C) (segid 3A4 and resid 160 and name O) 5.80 0.14 0.15
 assign (segid 3A4 and resid 158 and name C) (segid 3A4 and resid 161 and name C) 4.92 0.17 0.17
 assign (segid 3A4 and resid 158 and name C) (segid 3A4 and resid 161 and name CA) 4.79 0.30 0.29
 5 assign (segid 3A4 and resid 158 and name C) (segid 3A4 and resid 161 and name CB) 4.91 0.58 0.57
 assign (segid 3A4 and resid 158 and name C) (segid 3A4 and resid 161 and name N) 4.00 0.30 0.31
 assign (segid 3A4 and resid 158 and name C) (segid 3A4 and resid 161 and name O) 5.96 0.27 0.27
 assign (segid 3A4 and resid 158 and name CA) (segid 3A4 and resid 158 and name C) 1.52 0.01 0.01
 assign (segid 3A4 and resid 158 and name CA) (segid 3A4 and resid 158 and name CB) 1.52 0.01 0.01
 10 assign (segid 3A4 and resid 158 and name CA) (segid 3A4 and resid 158 and name O) 2.39 0.02 0.01
 assign (segid 3A4 and resid 158 and name CA) (segid 3A4 and resid 159 and name C) 4.45 0.05 0.05
 assign (segid 3A4 and resid 158 and name CA) (segid 3A4 and resid 159 and name CA) 3.80 0.01 0.02
 assign (segid 3A4 and resid 158 and name CA) (segid 3A4 and resid 159 and name CB) 4.87 0.02 0.03
 assign (segid 3A4 and resid 158 and name CA) (segid 3A4 and resid 159 and name N) 2.43 0.02 0.02
 15 assign (segid 3A4 and resid 158 and name CA) (segid 3A4 and resid 159 and name O) 5.33 0.13 0.13
 assign (segid 3A4 and resid 158 and name CA) (segid 3A4 and resid 160 and name C) 5.70 0.21 0.20
 assign (segid 3A4 and resid 158 and name CA) (segid 3A4 and resid 160 and name CA) 5.61 0.24 0.24
 assign (segid 3A4 and resid 158 and name CA) (segid 3A4 and resid 160 and name CB) 6.12 0.35 0.36
 assign (segid 3A4 and resid 158 and name CA) (segid 3A4 and resid 160 and name N) 4.49 0.23 0.23
 20 assign (segid 3A4 and resid 158 and name CA) (segid 3A4 and resid 160 and name O) 6.82 0.14 0.15
 assign (segid 3A4 and resid 158 and name CA) (segid 3A4 and resid 161 and name C) 5.70 0.23 0.22
 assign (segid 3A4 and resid 158 and name CA) (segid 3A4 and resid 161 and name CB) 5.13 0.57 0.57
 assign (segid 3A4 and resid 158 and name CA) (segid 3A4 and resid 161 and name N) 4.80 0.27 0.28
 25 assign (segid 3A4 and resid 158 and name CA) (segid 3A4 and resid 161 and name O) 6.62 0.43 0.44
 assign (segid 3A4 and resid 158 and name CA) (segid 3A4 and resid 187 and name CA) 9.74 2.04 2.03
 assign (segid 3A4 and resid 158 and name CA) (segid 3A4 and resid 187 and name CB) 9.96 2.22 2.22
 assign (segid 3A4 and resid 158 and name CA) (segid 3A4 and resid 188 and name CA) 12.88 1.83 1.83
 30 assign (segid 3A4 and resid 158 and name CA) (segid 3A4 and resid 189 and name CA) 12.88 1.79 1.78
 assign (segid 3A4 and resid 158 and name CA) (segid 3A4 and resid 189 and name CB) 13.00 2.07 2.07
 assign (segid 3A4 and resid 158 and name CA) (segid 3A4 and resid 190 and name CA) 9.76 1.55 1.56
 assign (segid 3A4 and resid 158 and name CA) (segid 3A4 and resid 190 and name CB) 8.40 1.62 1.61
 35 assign (segid 3A4 and resid 158 and name CA) (segid 3A4 and resid 191 and name CA) 11.17 1.11 1.10
 assign (segid 3A4 and resid 158 and name CA) (segid 3A4 and resid 191 and name CB) 11.65 1.07 1.06
 assign (segid 3A4 and resid 158 and name CA) (segid 3A4 and resid 192 and name CA) 14.34 1.19 1.18
 assign (segid 3A4 and resid 158 and name CA) (segid 3A4 and resid 192 and name CB) 15.11 1.26 1.26
 assign (segid 3A4 and resid 158 and name CA) (segid 3A4 and resid 193 and name CA) 13.41 1.25 1.24
 40 assign (segid 3A4 and resid 158 and name CA) (segid 3A4 and resid 193 and name CB) 12.53 1.37 1.36
 assign (segid 3A4 and resid 158 and name CA) (segid 3A4 and resid 194 and name CA) 12.32 1.06 1.05
 assign (segid 3A4 and resid 158 and name CA) (segid 3A4 and resid 194 and name CB) 11.25 1.00 1.00
 assign (segid 3A4 and resid 158 and name CA) (segid 3A4 and resid 195 and name CA) 15.38 0.82 0.83
 assign (segid 3A4 and resid 158 and name CA) (segid 3A4 and resid 195 and name CB) 15.76 0.80 0.81
 45 assign (segid 3A4 and resid 158 and name CA) (segid 3A4 and resid 196 and name CA) 17.46 1.02 1.02
 assign (segid 3A4 and resid 158 and name CA) (segid 3A4 and resid 196 and name CB) 17.45 1.11 1.10
 assign (segid 3A4 and resid 158 and name CA) (segid 3A4 and resid 197 and name CA) 16.64 1.28 1.29
 assign (segid 3A4 and resid 158 and name CA) (segid 3A4 and resid 197 and name CB) 15.38 1.48 1.47
 assign (segid 3A4 and resid 158 and name CA) (segid 3A4 and resid 198 and name CB) 16.81 0.98 0.98
 50 assign (segid 3A4 and resid 158 and name CA) (segid 3A4 and resid 246 and name CA) 17.81 0.60 0.61
 assign (segid 3A4 and resid 158 and name CA) (segid 3A4 and resid 246 and name CB) 18.57 0.62 0.62
 assign (segid 3A4 and resid 158 and name CA) (segid 3A4 and resid 248 and name CA) 17.24 1.15 1.16
 assign (segid 3A4 and resid 158 and name CA) (segid 3A4 and resid 249 and name CA) 13.96 0.95 0.96
 assign (segid 3A4 and resid 158 and name CA) (segid 3A4 and resid 250 and name CA) 14.40 0.84 0.84
 55 assign (segid 3A4 and resid 158 and name CA) (segid 3A4 and resid 250 and name CB) 15.59 0.76 0.76
 assign (segid 3A4 and resid 158 and name CA) (segid 3A4 and resid 251 and name CA) 15.56 1.32 1.32
 assign (segid 3A4 and resid 158 and name CA) (segid 3A4 and resid 251 and name CB) 16.76 1.37 1.37
 assign (segid 3A4 and resid 158 and name CA) (segid 3A4 and resid 252 and name CA) 12.70 1.59 1.60
 assign (segid 3A4 and resid 158 and name CA) (segid 3A4 and resid 252 and name CB) 12.38 1.56 1.56
 60 assign (segid 3A4 and resid 158 and name CA) (segid 3A4 and resid 253 and name CA) 10.16 1.32 1.32
 assign (segid 3A4 and resid 158 and name CA) (segid 3A4 and resid 254 and name CA) 12.76 1.22 1.23
 assign (segid 3A4 and resid 158 and name CA) (segid 3A4 and resid 255 and name CA) 13.86 1.87 1.88
 assign (segid 3A4 and resid 158 and name CA) (segid 3A4 and resid 256 and name CA) 11.34 2.44 2.44
 assign (segid 3A4 and resid 158 and name CA) (segid 3A4 and resid 257 and name CA) 9.82 2.42 2.42
 65 assign (segid 3A4 and resid 158 and name CA) (segid 3A4 and resid 258 and name CA) 13.07 2.10 2.09
 assign (segid 3A4 and resid 158 and name CA) (segid 3A4 and resid 258 and name CB) 13.86 1.87 1.86
 assign (segid 3A4 and resid 158 and name CA) (segid 3A4 and resid 260 and name CB) 12.02 3.04 3.03
 assign (segid 3A4 and resid 158 and name CA) (segid 3A4 and resid 261 and name CA) 13.72 2.44 2.43
 assign (segid 3A4 and resid 158 and name CA) (segid 3A4 and resid 318 and name CA) 16.40 1.66 1.65
 70 assign (segid 3A4 and resid 158 and name CA) (segid 3A4 and resid 318 and name CB) 15.86 1.84 1.85
 assign (segid 3A4 and resid 158 and name CA) (segid 3A4 and resid 319 and name CA) 16.23 1.45 1.45
 assign (segid 3A4 and resid 158 and name CA) (segid 3A4 and resid 319 and name CB) 16.43 1.28 1.27
 assign (segid 3A4 and resid 158 and name CA) (segid 3A4 and resid 427 and name CA) 14.65 2.54 2.54
 assign (segid 3A4 and resid 158 and name CA) (segid 3A4 and resid 428 and name CA) 14.34 1.84 1.85
 assign (segid 3A4 and resid 158 and name CA) (segid 3A4 and resid 429 and name CA) 13.67 2.48 2.47
 75 assign (segid 3A4 and resid 158 and name CA) (segid 3A4 and resid 430 and name CA) 13.92 2.83 2.83
 assign (segid 3A4 and resid 158 and name CA) (segid 3A4 and resid 431 and name CA) 13.04 1.90 1.90
 assign (segid 3A4 and resid 158 and name CA) (segid 3A4 and resid 433 and name CA) 13.96 2.13 2.13
 assign (segid 3A4 and resid 158 and name CA) (segid 3A4 and resid 434 and name CA) 13.68 2.22 2.22
 assign (segid 3A4 and resid 158 and name CA) (segid 3A4 and resid 436 and name CA) 13.58 3.11 3.10
 80 assign (segid 3A4 and resid 158 and name CB) (segid 3A4 and resid 159 and name C) 5.45 0.05 0.05
 assign (segid 3A4 and resid 158 and name CB) (segid 3A4 and resid 159 and name CA) 4.46 0.06 0.06
 assign (segid 3A4 and resid 158 and name CB) (segid 3A4 and resid 159 and name CB) 5.34 0.09 0.08
 assign (segid 3A4 and resid 158 and name CB) (segid 3A4 and resid 159 and name N) 3.15 0.06 0.05
 assign (segid 3A4 and resid 158 and name CB) (segid 3A4 and resid 159 and name O) 6.30 0.14 0.13

	assign (segid 3A4 and resid 158 and name CB)	(segid 3A4 and resid 160 and name C)	7.07	0.19	0.18
	assign (segid 3A4 and resid 158 and name CB)	(segid 3A4 and resid 160 and name CB)	6.93	0.18	0.17
	assign (segid 3A4 and resid 158 and name CB)	(segid 3A4 and resid 160 and name CB)	7.50	0.25	0.24
	assign (segid 3A4 and resid 158 and name CB)	(segid 3A4 and resid 160 and name N)	5.69	0.15	0.16
5	assign (segid 3A4 and resid 158 and name CB)	(segid 3A4 and resid 161 and name C)	6.82	0.22	0.22
	assign (segid 3A4 and resid 158 and name CB)	(segid 3A4 and resid 161 and name CA)	6.73	0.31	0.30
	assign (segid 3A4 and resid 158 and name CB)	(segid 3A4 and resid 161 and name CB)	6.39	0.63	0.62
	assign (segid 3A4 and resid 158 and name CB)	(segid 3A4 and resid 161 and name N)	6.19	0.28	0.28
	assign (segid 3A4 and resid 158 and name CB)	(segid 3A4 and resid 187 and name CA)	10.07	2.67	2.67
10	assign (segid 3A4 and resid 158 and name CB)	(segid 3A4 and resid 187 and name CB)	10.38	2.88	2.89
	assign (segid 3A4 and resid 158 and name CB)	(segid 3A4 and resid 188 and name CA)	13.21	2.45	2.45
	assign (segid 3A4 and resid 158 and name CB)	(segid 3A4 and resid 189 and name CA)	12.97	2.31	2.30
	assign (segid 3A4 and resid 158 and name CB)	(segid 3A4 and resid 189 and name CB)	12.99	2.57	2.57
	assign (segid 3A4 and resid 158 and name CB)	(segid 3A4 and resid 190 and name CA)	9.95	1.89	1.88
15	assign (segid 3A4 and resid 158 and name CB)	(segid 3A4 and resid 190 and name CB)	8.62	1.95	1.94
	assign (segid 3A4 and resid 158 and name CB)	(segid 3A4 and resid 191 and name CA)	11.63	1.48	1.48
	assign (segid 3A4 and resid 158 and name CB)	(segid 3A4 and resid 191 and name CB)	12.17	1.58	1.58
	assign (segid 3A4 and resid 158 and name CB)	(segid 3A4 and resid 192 and name CA)	14.60	1.55	1.56
	assign (segid 3A4 and resid 158 and name CB)	(segid 3A4 and resid 192 and name CB)	15.33	1.74	1.73
20	assign (segid 3A4 and resid 158 and name CB)	(segid 3A4 and resid 193 and name CA)	13.51	1.32	1.32
	assign (segid 3A4 and resid 158 and name CB)	(segid 3A4 and resid 193 and name CB)	12.55	1.43	1.44
	assign (segid 3A4 and resid 158 and name CB)	(segid 3A4 and resid 194 and name CA)	12.62	0.85	0.84
	assign (segid 3A4 and resid 158 and name CB)	(segid 3A4 and resid 194 and name CB)	11.66	0.74	0.74
	assign (segid 3A4 and resid 158 and name CB)	(segid 3A4 and resid 195 and name CA)	15.76	0.79	0.79
25	assign (segid 3A4 and resid 158 and name CB)	(segid 3A4 and resid 195 and name CB)	16.18	0.95	0.94
	assign (segid 3A4 and resid 158 and name CB)	(segid 3A4 and resid 196 and name CA)	17.62	0.92	0.93
	assign (segid 3A4 and resid 158 and name CB)	(segid 3A4 and resid 197 and name CA)	16.74	0.95	0.95
	assign (segid 3A4 and resid 158 and name CB)	(segid 3A4 and resid 197 and name CB)	15.47	1.14	1.14
	assign (segid 3A4 and resid 158 and name CB)	(segid 3A4 and resid 198 and name CA)	17.78	0.66	0.67
30	assign (segid 3A4 and resid 158 and name CB)	(segid 3A4 and resid 198 and name CB)	17.20	0.54	0.53
	assign (segid 3A4 and resid 158 and name CB)	(segid 3A4 and resid 248 and name CA)	17.91	0.93	0.93
	assign (segid 3A4 and resid 158 and name CB)	(segid 3A4 and resid 248 and name CB)	18.29	1.04	1.03
	assign (segid 3A4 and resid 158 and name CB)	(segid 3A4 and resid 249 and name CA)	14.72	0.74	0.74
	assign (segid 3A4 and resid 158 and name CB)	(segid 3A4 and resid 250 and name CA)	15.33	0.59	0.60
35	assign (segid 3A4 and resid 158 and name CB)	(segid 3A4 and resid 250 and name CB)	16.54	0.53	0.54
	assign (segid 3A4 and resid 158 and name CB)	(segid 3A4 and resid 251 and name CA)	16.36	1.12	1.11
	assign (segid 3A4 and resid 158 and name CB)	(segid 3A4 and resid 251 and name CB)	17.50	1.18	1.17
	assign (segid 3A4 and resid 158 and name CB)	(segid 3A4 and resid 252 and name CA)	13.38	1.43	1.44
	assign (segid 3A4 and resid 158 and name CB)	(segid 3A4 and resid 252 and name CB)	13.01	1.37	1.37
40	assign (segid 3A4 and resid 158 and name CB)	(segid 3A4 and resid 253 and name CA)	11.08	1.12	1.12
	assign (segid 3A4 and resid 158 and name CB)	(segid 3A4 and resid 254 and name CA)	13.73	1.10	1.11
	assign (segid 3A4 and resid 158 and name CB)	(segid 3A4 and resid 255 and name CA)	14.59	1.88	1.88
	assign (segid 3A4 and resid 158 and name CB)	(segid 3A4 and resid 256 and name CA)	11.90	2.53	2.52
	assign (segid 3A4 and resid 158 and name CB)	(segid 3A4 and resid 257 and name CA)	10.53	2.54	2.55
45	assign (segid 3A4 and resid 158 and name CB)	(segid 3A4 and resid 258 and name CA)	13.82	2.25	2.25
	assign (segid 3A4 and resid 158 and name CB)	(segid 3A4 and resid 258 and name CB)	14.68	1.98	1.98
	assign (segid 3A4 and resid 158 and name CB)	(segid 3A4 and resid 319 and name CA)	17.26	1.57	1.57
	assign (segid 3A4 and resid 158 and name CB)	(segid 3A4 and resid 319 and name CB)	17.47	1.37	1.37
	assign (segid 3A4 and resid 158 and name CB)	(segid 3A4 and resid 428 and name CA)	14.93	2.21	2.20
50	assign (segid 3A4 and resid 158 and name CB)	(segid 3A4 and resid 431 and name CA)	14.16	1.85	1.85
	assign (segid 3A4 and resid 158 and name CB)	(segid 3A4 and resid 433 and name CA)	14.71	2.37	2.38
	assign (segid 3A4 and resid 158 and name CB)	(segid 3A4 and resid 434 and name CA)	14.16	2.61	2.60
	assign (segid 3A4 and resid 158 and name N)	(segid 3A4 and resid 158 and name C)	2.45	0.03	0.02
	assign (segid 3A4 and resid 158 and name N)	(segid 3A4 and resid 158 and name CB)	1.45	0.00	0.01
55	assign (segid 3A4 and resid 158 and name N)	(segid 3A4 and resid 158 and name O)	2.44	0.02	0.03
	assign (segid 3A4 and resid 158 and name N)	(segid 3A4 and resid 159 and name C)	3.47	0.05	0.05
	assign (segid 3A4 and resid 158 and name N)	(segid 3A4 and resid 159 and name CA)	4.21	0.06	0.06
	assign (segid 3A4 and resid 158 and name N)	(segid 3A4 and resid 159 and name CB)	5.00	0.12	0.12
60	assign (segid 3A4 and resid 158 and name N)	(segid 3A4 and resid 159 and name N)	2.81	0.06	0.05
	assign (segid 3A4 and resid 158 and name N)	(segid 3A4 and resid 159 and name O)	5.79	0.11	0.11
	assign (segid 3A4 and resid 158 and name N)	(segid 3A4 and resid 160 and name C)	5.82	0.11	0.11
	assign (segid 3A4 and resid 158 and name N)	(segid 3A4 and resid 160 and name CA)	5.51	0.21	0.21
	assign (segid 3A4 and resid 158 and name N)	(segid 3A4 and resid 160 and name CB)	5.69	0.33	0.34
65	assign (segid 3A4 and resid 158 and name N)	(segid 3A4 and resid 160 and name N)	4.44	0.21	0.21
	assign (segid 3A4 and resid 158 and name N)	(segid 3A4 and resid 160 and name O)	7.01	0.09	0.10
	assign (segid 3A4 and resid 158 and name N)	(segid 3A4 and resid 161 and name C)	6.38	0.44	0.44
	assign (segid 3A4 and resid 158 and name N)	(segid 3A4 and resid 161 and name CA)	5.83	0.21	0.21
	assign (segid 3A4 and resid 158 and name N)	(segid 3A4 and resid 161 and name CB)	5.51	0.34	0.35
70	assign (segid 3A4 and resid 158 and name N)	(segid 3A4 and resid 161 and name N)	5.04	0.15	0.14
	assign (segid 3A4 and resid 158 and name N)	(segid 3A4 and resid 161 and name O)	7.34	0.71	0.70
	assign (segid 3A4 and resid 158 and name O)	(segid 3A4 and resid 158 and name CB)	3.29	0.04	0.05
	assign (segid 3A4 and resid 158 and name O)	(segid 3A4 and resid 159 and name C)	3.00	0.09	0.10
	assign (segid 3A4 and resid 158 and name O)	(segid 3A4 and resid 159 and name CA)	2.76	0.04	0.03
75	assign (segid 3A4 and resid 158 and name O)	(segid 3A4 and resid 159 and name CB)	4.24	0.06	0.06
	assign (segid 3A4 and resid 158 and name O)	(segid 3A4 and resid 159 and name N)	2.25	0.01	0.00
	assign (segid 3A4 and resid 158 and name O)	(segid 3A4 and resid 159 and name O)	3.46	0.19	0.20
	assign (segid 3A4 and resid 158 and name O)	(segid 3A4 and resid 160 and name C)	4.28	0.33	0.32
	assign (segid 3A4 and resid 158 and name O)	(segid 3A4 and resid 160 and name CA)	4.48	0.28	0.28
80	assign (segid 3A4 and resid 158 and name O)	(segid 3A4 and resid 160 and name CB)	5.51	0.35	0.35
	assign (segid 3A4 and resid 158 and name O)	(segid 3A4 and resid 160 and name N)	3.50	0.25	0.25
	assign (segid 3A4 and resid 158 and name O)	(segid 3A4 and resid 160 and name O)	5.23	0.25	0.24
	assign (segid 3A4 and resid 158 and name O)	(segid 3A4 and resid 161 and name C)	3.93	0.26	0.25

	assign (segid 3A4 and resid 158 and name O) (segid 3A4 and resid 161 and name CA)	4.03	0.49	0.49
	assign (segid 3A4 and resid 158 and name O) (segid 3A4 and resid 161 and name CB)	4.29	0.80	0.80
	assign (segid 3A4 and resid 158 and name O) (segid 3A4 and resid 161 and name N)	3.49	0.49	0.48
	assign (segid 3A4 and resid 158 and name O) (segid 3A4 and resid 161 and name O)	4.94	0.19	0.19
	assign (segid 3A4 and resid 159 and name C) (segid 3A4 and resid 159 and name CB)	2.49	0.04	0.04
5	assign (segid 3A4 and resid 159 and name C) (segid 3A4 and resid 159 and name O)	1.24	0.01	0.01
	assign (segid 3A4 and resid 159 and name C) (segid 3A4 and resid 160 and name C)	3.07	0.08	0.08
	assign (segid 3A4 and resid 159 and name C) (segid 3A4 and resid 160 and name CA)	2.43	0.02	0.01
	assign (segid 3A4 and resid 159 and name C) (segid 3A4 and resid 160 and name CB)	3.71	0.02	0.02
	assign (segid 3A4 and resid 159 and name C) (segid 3A4 and resid 160 and name N)	1.33	0.00	0.00
10	assign (segid 3A4 and resid 159 and name C) (segid 3A4 and resid 160 and name O)	3.96	0.13	0.13
	assign (segid 3A4 and resid 159 and name C) (segid 3A4 and resid 161 and name C)	4.73	0.15	0.14
	assign (segid 3A4 and resid 159 and name C) (segid 3A4 and resid 161 and name CA)	4.54	0.12	0.13
	assign (segid 3A4 and resid 159 and name C) (segid 3A4 and resid 161 and name CB)	5.45	0.22	0.23
	assign (segid 3A4 and resid 159 and name C) (segid 3A4 and resid 161 and name N)	3.32	0.11	0.11
15	assign (segid 3A4 and resid 159 and name C) (segid 3A4 and resid 161 and name O)	5.86	0.15	0.16
	assign (segid 3A4 and resid 159 and name CA) (segid 3A4 and resid 159 and name C)	1.52	0.01	0.01
	assign (segid 3A4 and resid 159 and name CA) (segid 3A4 and resid 159 and name CB)	1.53	0.02	0.01
	assign (segid 3A4 and resid 159 and name CA) (segid 3A4 and resid 159 and name O)	2.39	0.02	0.02
	assign (segid 3A4 and resid 159 and name CA) (segid 3A4 and resid 160 and name C)	4.47	0.06	0.06
20	assign (segid 3A4 and resid 159 and name CA) (segid 3A4 and resid 160 and name CA)	3.81	0.02	0.02
	assign (segid 3A4 and resid 159 and name CA) (segid 3A4 and resid 160 and name CB)	4.88	0.04	0.03
	assign (segid 3A4 and resid 159 and name CA) (segid 3A4 and resid 160 and name N)	2.44	0.03	0.03
	assign (segid 3A4 and resid 159 and name CA) (segid 3A4 and resid 160 and name O)	5.43	0.12	0.12
	assign (segid 3A4 and resid 159 and name CA) (segid 3A4 and resid 161 and name C)	5.62	0.15	0.15
25	assign (segid 3A4 and resid 159 and name CA) (segid 3A4 and resid 161 and name CA)	5.55	0.13	0.14
	assign (segid 3A4 and resid 159 and name CA) (segid 3A4 and resid 161 and name CB)	6.22	0.31	0.31
	assign (segid 3A4 and resid 159 and name CA) (segid 3A4 and resid 161 and name N)	4.43	0.11	0.12
	assign (segid 3A4 and resid 159 and name CA) (segid 3A4 and resid 161 and name O)	6.73	0.18	0.19
	assign (segid 3A4 and resid 159 and name CA) (segid 3A4 and resid 161 and name O)	7.51	1.82	1.83
30	assign (segid 3A4 and resid 159 and name CA) (segid 3A4 and resid 187 and name CA)	7.71	1.87	1.86
	assign (segid 3A4 and resid 159 and name CA) (segid 3A4 and resid 187 and name CB)	10.72	1.70	1.69
	assign (segid 3A4 and resid 159 and name CA) (segid 3A4 and resid 188 and name CA)	11.01	1.88	1.88
	assign (segid 3A4 and resid 159 and name CA) (segid 3A4 and resid 189 and name CA)	11.16	2.15	2.16
	assign (segid 3A4 and resid 159 and name CA) (segid 3A4 and resid 189 and name CB)	8.23	1.81	1.81
35	assign (segid 3A4 and resid 159 and name CA) (segid 3A4 and resid 190 and name CA)	6.81	1.87	1.87
	assign (segid 3A4 and resid 159 and name CA) (segid 3A4 and resid 190 and name CB)	9.62	1.34	1.34
	assign (segid 3A4 and resid 159 and name CA) (segid 3A4 and resid 191 and name CA)	9.92	1.25	1.25
	assign (segid 3A4 and resid 159 and name CA) (segid 3A4 and resid 191 and name CB)	12.88	1.44	1.43
	assign (segid 3A4 and resid 159 and name CA) (segid 3A4 and resid 192 and name CA)	13.53	1.43	1.43
40	assign (segid 3A4 and resid 159 and name CA) (segid 3A4 and resid 192 and name CB)	12.43	1.62	1.62
	assign (segid 3A4 and resid 159 and name CA) (segid 3A4 and resid 193 and name CA)	11.59	1.75	1.76
	assign (segid 3A4 and resid 159 and name CA) (segid 3A4 and resid 193 and name CB)	11.76	1.25	1.26
	assign (segid 3A4 and resid 159 and name CA) (segid 3A4 and resid 194 and name CA)	10.71	1.14	1.14
	assign (segid 3A4 and resid 159 and name CA) (segid 3A4 and resid 194 and name CB)	14.52	1.07	1.07
45	assign (segid 3A4 and resid 159 and name CA) (segid 3A4 and resid 195 and name CA)	14.68	1.08	1.08
	assign (segid 3A4 and resid 159 and name CA) (segid 3A4 and resid 195 and name CB)	16.68	1.32	1.31
	assign (segid 3A4 and resid 159 and name CA) (segid 3A4 and resid 196 and name CA)	16.60	1.44	1.44
	assign (segid 3A4 and resid 159 and name CA) (segid 3A4 and resid 196 and name CB)	15.33	1.66	1.66
	assign (segid 3A4 and resid 159 and name CA) (segid 3A4 and resid 197 and name CA)	16.63	0.92	0.91
50	assign (segid 3A4 and resid 159 and name CA) (segid 3A4 and resid 198 and name CB)	17.10	1.30	1.29
	assign (segid 3A4 and resid 159 and name CA) (segid 3A4 and resid 246 and name CA)	17.41	1.11	1.12
	assign (segid 3A4 and resid 159 and name CA) (segid 3A4 and resid 248 and name CA)	17.85	1.18	1.18
	assign (segid 3A4 and resid 159 and name CA) (segid 3A4 and resid 248 and name CB)	13.89	1.12	1.12
	assign (segid 3A4 and resid 159 and name CA) (segid 3A4 and resid 249 and name CA)	14.43	1.15	1.15
55	assign (segid 3A4 and resid 159 and name CA) (segid 3A4 and resid 250 and name CA)	15.48	1.25	1.25
	assign (segid 3A4 and resid 159 and name CA) (segid 3A4 and resid 250 and name CB)	16.26	0.96	0.95
	assign (segid 3A4 and resid 159 and name CA) (segid 3A4 and resid 251 and name CA)	17.48	0.97	0.98
	assign (segid 3A4 and resid 159 and name CA) (segid 3A4 and resid 251 and name CB)	13.73	1.05	1.06
	assign (segid 3A4 and resid 159 and name CA) (segid 3A4 and resid 252 and name CA)	13.28	1.14	1.14
60	assign (segid 3A4 and resid 159 and name CA) (segid 3A4 and resid 252 and name CB)	11.00	0.92	0.93
	assign (segid 3A4 and resid 159 and name CA) (segid 3A4 and resid 253 and name CA)	13.67	0.88	0.89
	assign (segid 3A4 and resid 159 and name CA) (segid 3A4 and resid 254 and name CA)	15.36	0.88	0.88
	assign (segid 3A4 and resid 159 and name CA) (segid 3A4 and resid 255 and name CA)	13.40	1.37	1.37
	assign (segid 3A4 and resid 159 and name CA) (segid 3A4 and resid 256 and name CA)	11.90	1.36	1.36
65	assign (segid 3A4 and resid 159 and name CA) (segid 3A4 and resid 257 and name CA)	14.88	0.95	0.95
	assign (segid 3A4 and resid 159 and name CA) (segid 3A4 and resid 258 and name CA)	15.46	0.74	0.74
	assign (segid 3A4 and resid 159 and name CA) (segid 3A4 and resid 258 and name CB)	14.63	1.94	1.95
	assign (segid 3A4 and resid 159 and name CA) (segid 3A4 and resid 260 and name CB)	16.01	1.38	1.37
	assign (segid 3A4 and resid 159 and name CA) (segid 3A4 and resid 261 and name CA)	17.71	0.84	0.85
70	assign (segid 3A4 and resid 159 and name CA) (segid 3A4 and resid 318 and name CA)	17.35	0.80	0.80
	assign (segid 3A4 and resid 159 and name CA) (segid 3A4 and resid 318 and name CB)	17.00	1.19	1.20
	assign (segid 3A4 and resid 159 and name CA) (segid 3A4 and resid 319 and name CA)	17.18	1.15	1.14
	assign (segid 3A4 and resid 159 and name CA) (segid 3A4 and resid 319 and name CB)	15.81	2.17	2.18
	assign (segid 3A4 and resid 159 and name CA) (segid 3A4 and resid 427 and name CA)	14.91	1.68	1.67
75	assign (segid 3A4 and resid 159 and name CA) (segid 3A4 and resid 428 and name CA)	13.98	3.05	3.04
	assign (segid 3A4 and resid 159 and name CA) (segid 3A4 and resid 430 and name CA)	13.01	2.28	2.27
	assign (segid 3A4 and resid 159 and name CA) (segid 3A4 and resid 431 and name CA)	15.20	1.61	1.61
	assign (segid 3A4 and resid 159 and name CA) (segid 3A4 and resid 433 and name CA)	15.54	1.59	1.60
	assign (segid 3A4 and resid 159 and name CA) (segid 3A4 and resid 434 and name CA)	5.46	0.12	0.13
80	assign (segid 3A4 and resid 159 and name CB) (segid 3A4 and resid 160 and name C)	4.46	0.13	0.13
	assign (segid 3A4 and resid 159 and name CB) (segid 3A4 and resid 160 and name CA)	5.31	0.16	0.17
	assign (segid 3A4 and resid 159 and name CB) (segid 3A4 and resid 160 and name CB)	3.15	0.13	0.14

	assign (segid 3A4 and resid 159 and name CB)	(segid 3A4 and resid 160 and name O)	6.37	0.17	0.17
	assign (segid 3A4 and resid 159 and name CB)	(segid 3A4 and resid 161 and name C)	7.03	0.16	0.16
	assign (segid 3A4 and resid 159 and name CB)	(segid 3A4 and resid 161 and name CA)	6.89	0.13	0.14
	assign (segid 3A4 and resid 159 and name CB)	(segid 3A4 and resid 161 and name CB)	7.59	0.26	0.26
5	assign (segid 3A4 and resid 159 and name CB)	(segid 3A4 and resid 161 and name N)	5.65	0.12	0.12
	assign (segid 3A4 and resid 159 and name CB)	(segid 3A4 and resid 187 and name CA)	7.23	1.96	1.97
	assign (segid 3A4 and resid 159 and name CB)	(segid 3A4 and resid 187 and name CB)	7.65	1.94	1.94
	assign (segid 3A4 and resid 159 and name CB)	(segid 3A4 and resid 188 and name CA)	10.19	1.87	1.87
	assign (segid 3A4 and resid 159 and name CB)	(segid 3A4 and resid 189 and name CA)	10.19	2.15	2.16
	assign (segid 3A4 and resid 159 and name CB)	(segid 3A4 and resid 189 and name CB)	10.33	2.45	2.46
10	assign (segid 3A4 and resid 159 and name CB)	(segid 3A4 and resid 190 and name CA)	7.39	2.04	2.04
	assign (segid 3A4 and resid 159 and name CB)	(segid 3A4 and resid 190 and name CB)	6.06	2.08	2.08
	assign (segid 3A4 and resid 159 and name CB)	(segid 3A4 and resid 191 and name CA)	8.94	1.55	1.54
	assign (segid 3A4 and resid 159 and name CB)	(segid 3A4 and resid 191 and name CB)	9.34	1.50	1.49
	assign (segid 3A4 and resid 159 and name CB)	(segid 3A4 and resid 192 and name CA)	12.02	1.63	1.64
15	assign (segid 3A4 and resid 159 and name CB)	(segid 3A4 and resid 192 and name CB)	12.67	1.65	1.64
	assign (segid 3A4 and resid 159 and name CB)	(segid 3A4 and resid 193 and name CA)	11.47	1.78	1.79
	assign (segid 3A4 and resid 159 and name CB)	(segid 3A4 and resid 193 and name CB)	10.61	1.94	1.95
	assign (segid 3A4 and resid 159 and name CB)	(segid 3A4 and resid 194 and name CA)	10.97	1.30	1.31
20	assign (segid 3A4 and resid 159 and name CB)	(segid 3A4 and resid 194 and name CB)	10.01	1.19	1.19
	assign (segid 3A4 and resid 159 and name CB)	(segid 3A4 and resid 195 and name CA)	13.72	1.22	1.22
	assign (segid 3A4 and resid 159 and name CB)	(segid 3A4 and resid 195 and name CB)	13.90	1.27	1.27
	assign (segid 3A4 and resid 159 and name CB)	(segid 3A4 and resid 196 and name CA)	15.74	1.43	1.43
	assign (segid 3A4 and resid 159 and name CB)	(segid 3A4 and resid 196 and name CB)	15.62	1.58	1.57
25	assign (segid 3A4 and resid 159 and name CB)	(segid 3A4 and resid 197 and name CA)	15.59	1.48	1.48
	assign (segid 3A4 and resid 159 and name CB)	(segid 3A4 and resid 197 and name CB)	14.49	1.65	1.65
	assign (segid 3A4 and resid 159 and name CB)	(segid 3A4 and resid 198 and name CA)	16.62	1.04	1.04
	assign (segid 3A4 and resid 159 and name CB)	(segid 3A4 and resid 198 and name CB)	15.93	0.96	0.95
	assign (segid 3A4 and resid 159 and name CB)	(segid 3A4 and resid 246 and name CA)	16.65	1.77	1.78
30	assign (segid 3A4 and resid 159 and name CB)	(segid 3A4 and resid 248 and name CA)	17.04	1.41	1.40
	assign (segid 3A4 and resid 159 and name CB)	(segid 3A4 and resid 248 and name CB)	17.39	1.37	1.37
	assign (segid 3A4 and resid 159 and name CB)	(segid 3A4 and resid 249 and name CA)	13.53	1.47	1.46
	assign (segid 3A4 and resid 159 and name CB)	(segid 3A4 and resid 250 and name CA)	14.32	1.72	1.71
	assign (segid 3A4 and resid 159 and name CB)	(segid 3A4 and resid 250 and name CB)	15.38	1.85	1.85
35	assign (segid 3A4 and resid 159 and name CB)	(segid 3A4 and resid 251 and name CA)	16.20	1.36	1.37
	assign (segid 3A4 and resid 159 and name CB)	(segid 3A4 and resid 251 and name CB)	17.37	1.34	1.34
	assign (segid 3A4 and resid 159 and name CB)	(segid 3A4 and resid 252 and name CA)	13.65	1.19	1.19
	assign (segid 3A4 and resid 159 and name CB)	(segid 3A4 and resid 252 and name CB)	13.09	1.22	1.22
	assign (segid 3A4 and resid 159 and name CB)	(segid 3A4 and resid 253 and name CA)	11.13	1.28	1.28
40	assign (segid 3A4 and resid 159 and name CB)	(segid 3A4 and resid 254 and name CA)	13.98	1.43	1.43
	assign (segid 3A4 and resid 159 and name CB)	(segid 3A4 and resid 255 and name CA)	15.64	1.03	1.04
	assign (segid 3A4 and resid 159 and name CB)	(segid 3A4 and resid 256 and name CA)	13.77	1.13	1.13
	assign (segid 3A4 and resid 159 and name CB)	(segid 3A4 and resid 257 and name CA)	12.56	1.03	1.03
	assign (segid 3A4 and resid 159 and name CB)	(segid 3A4 and resid 258 and name CA)	15.60	0.85	0.84
45	assign (segid 3A4 and resid 159 and name CB)	(segid 3A4 and resid 258 and name CB)	16.13	0.87	0.87
	assign (segid 3A4 and resid 159 and name CB)	(segid 3A4 and resid 259 and name CA)	17.88	0.81	0.81
	assign (segid 3A4 and resid 159 and name CB)	(segid 3A4 and resid 259 and name CB)	18.18	0.94	0.94
	assign (segid 3A4 and resid 159 and name CB)	(segid 3A4 and resid 260 and name CA)	16.56	1.24	1.24
	assign (segid 3A4 and resid 159 and name CB)	(segid 3A4 and resid 260 and name CB)	15.30	1.44	1.44
50	assign (segid 3A4 and resid 159 and name CB)	(segid 3A4 and resid 261 and name CA)	16.89	0.95	0.94
	assign (segid 3A4 and resid 159 and name CB)	(segid 3A4 and resid 318 and name CB)	18.27	0.75	0.75
	assign (segid 3A4 and resid 159 and name CB)	(segid 3A4 and resid 427 and name CA)	16.96	1.90	1.90
	assign (segid 3A4 and resid 159 and name CB)	(segid 3A4 and resid 428 and name CA)	16.02	1.57	1.57
	assign (segid 3A4 and resid 159 and name CB)	(segid 3A4 and resid 431 and name CA)	13.97	2.66	2.65
55	assign (segid 3A4 and resid 159 and name CB)	(segid 3A4 and resid 433 and name CA)	16.31	1.56	1.55
	assign (segid 3A4 and resid 159 and name CB)	(segid 3A4 and resid 434 and name CA)	16.64	1.36	1.35
	assign (segid 3A4 and resid 159 and name N)	(segid 3A4 and resid 159 and name C)	2.47	0.02	0.02
	assign (segid 3A4 and resid 159 and name N)	(segid 3A4 and resid 159 and name CA)	1.46	0.01	0.00
	assign (segid 3A4 and resid 159 and name N)	(segid 3A4 and resid 159 and name CB)	2.47	0.03	0.02
60	assign (segid 3A4 and resid 159 and name N)	(segid 3A4 and resid 159 and name O)	3.49	0.08	0.08
	assign (segid 3A4 and resid 159 and name N)	(segid 3A4 and resid 160 and name C)	4.80	0.04	0.05
	assign (segid 3A4 and resid 159 and name N)	(segid 3A4 and resid 160 and name CA)	4.27	0.07	0.07
	assign (segid 3A4 and resid 159 and name N)	(segid 3A4 and resid 160 and name CB)	5.06	0.10	0.11
	assign (segid 3A4 and resid 159 and name N)	(segid 3A4 and resid 160 and name N)	2.86	0.08	0.09
65	assign (segid 3A4 and resid 159 and name N)	(segid 3A4 and resid 160 and name O)	5.91	0.07	0.07
	assign (segid 3A4 and resid 159 and name N)	(segid 3A4 and resid 161 and name C)	5.67	0.19	0.18
	assign (segid 3A4 and resid 159 and name N)	(segid 3A4 and resid 161 and name CA)	5.46	0.12	0.13
	assign (segid 3A4 and resid 159 and name N)	(segid 3A4 and resid 161 and name CB)	5.79	0.33	0.34
	assign (segid 3A4 and resid 159 and name N)	(segid 3A4 and resid 161 and name N)	4.42	0.11	0.10
70	assign (segid 3A4 and resid 159 and name N)	(segid 3A4 and resid 161 and name O)	6.78	0.31	0.30
	assign (segid 3A4 and resid 159 and name O)	(segid 3A4 and resid 159 and name CB)	3.27	0.05	0.06
	assign (segid 3A4 and resid 159 and name O)	(segid 3A4 and resid 160 and name C)	3.03	0.14	0.14
	assign (segid 3A4 and resid 159 and name O)	(segid 3A4 and resid 160 and name CA)	2.75	0.03	0.02
	assign (segid 3A4 and resid 159 and name O)	(segid 3A4 and resid 160 and name CB)	4.23	0.03	0.03
75	assign (segid 3A4 and resid 159 and name O)	(segid 3A4 and resid 160 and name N)	2.25	0.02	0.01
	assign (segid 3A4 and resid 159 and name O)	(segid 3A4 and resid 160 and name O)	3.58	0.21	0.21
	assign (segid 3A4 and resid 159 and name O)	(segid 3A4 and resid 161 and name C)	4.38	0.29	0.28
	assign (segid 3A4 and resid 159 and name O)	(segid 3A4 and resid 161 and name CB)	4.47	0.22	0.22
	assign (segid 3A4 and resid 159 and name O)	(segid 3A4 and resid 161 and name N)	5.61	0.29	0.28
80	assign (segid 3A4 and resid 159 and name O)	(segid 3A4 and resid 161 and name O)	3.46	0.17	0.17
	assign (segid 3A4 and resid 159 and name O)	(segid 3A4 and resid 161 and name O)	5.42	0.27	0.28
	assign (segid 3A4 and resid 160 and name C)	(segid 3A4 and resid 160 and name CB)	2.51	0.03	0.03
	assign (segid 3A4 and resid 160 and name C)	(segid 3A4 and resid 160 and name O)	1.24	0.01	0.01

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	assign (segid 3A4 and resid 160 and name CB) (segid 3A4 and resid 194 and name CA)	11.02	2.74	2.74
	assign (segid 3A4 and resid 160 and name CB) (segid 3A4 and resid 194 and name CB)	9.71	2.72	2.73
	assign (segid 3A4 and resid 160 and name CB) (segid 3A4 and resid 246 and name CA)	14.82	1.67	1.68
	assign (segid 3A4 and resid 160 and name CB) (segid 3A4 and resid 246 and name CB)	15.38	1.53	1.53
5	assign (segid 3A4 and resid 160 and name CB) (segid 3A4 and resid 249 and name CA)	11.70	1.86	1.87
	assign (segid 3A4 and resid 160 and name CB) (segid 3A4 and resid 250 and name CA)	11.79	1.62	1.62
	assign (segid 3A4 and resid 160 and name CB) (segid 3A4 and resid 250 and name CB)	12.76	1.61	1.61
	assign (segid 3A4 and resid 160 and name CB) (segid 3A4 and resid 251 and name CA)	13.80	1.58	1.57
	assign (segid 3A4 and resid 160 and name CB) (segid 3A4 and resid 251 and name CB)	15.08	1.58	1.58
10	assign (segid 3A4 and resid 160 and name CB) (segid 3A4 and resid 252 and name CA)	11.73	1.63	1.63
	assign (segid 3A4 and resid 160 and name CB) (segid 3A4 and resid 252 and name CB)	11.44	1.73	1.74
	assign (segid 3A4 and resid 160 and name CB) (segid 3A4 and resid 253 and name CA)	8.72	1.57	1.58
	assign (segid 3A4 and resid 160 and name CB) (segid 3A4 and resid 254 and name CA)	11.04	1.63	1.64
	assign (segid 3A4 and resid 160 and name CB) (segid 3A4 and resid 255 and name CA)	13.18	1.58	1.58
15	assign (segid 3A4 and resid 160 and name CB) (segid 3A4 and resid 256 and name CA)	11.89	1.72	1.72
	assign (segid 3A4 and resid 160 and name CB) (segid 3A4 and resid 257 and name CA)	10.33	2.00	2.01
	assign (segid 3A4 and resid 160 and name CB) (segid 3A4 and resid 258 and name CA)	12.95	1.97	1.97
	assign (segid 3A4 and resid 160 and name CB) (segid 3A4 and resid 258 and name CB)	13.28	1.85	1.85
	assign (segid 3A4 and resid 160 and name CB) (segid 3A4 and resid 259 and name CA)	15.72	1.60	1.79
20	assign (segid 3A4 and resid 160 and name CB) (segid 3A4 and resid 259 and name CB)	16.10	1.78	1.78
	assign (segid 3A4 and resid 160 and name CB) (segid 3A4 and resid 260 and name CA)	15.06	1.87	1.88
	assign (segid 3A4 and resid 160 and name CB) (segid 3A4 and resid 260 and name CB)	13.99	1.93	1.92
	assign (segid 3A4 and resid 160 and name CB) (segid 3A4 and resid 261 and name CA)	15.07	1.97	1.97
	assign (segid 3A4 and resid 160 and name CB) (segid 3A4 and resid 318 and name CB)	15.53	1.74	1.74
25	assign (segid 3A4 and resid 160 and name CB) (segid 3A4 and resid 319 and name CA)	14.65	2.01	2.01
	assign (segid 3A4 and resid 160 and name CB) (segid 3A4 and resid 319 and name CB)	14.67	2.01	2.01
	assign (segid 3A4 and resid 160 and name CB) (segid 3A4 and resid 427 and name CA)	15.73	1.31	1.31
	assign (segid 3A4 and resid 160 and name CB) (segid 3A4 and resid 428 and name CA)	14.67	2.05	2.06
	assign (segid 3A4 and resid 160 and name CB) (segid 3A4 and resid 429 and name CA)	13.24	3.35	3.35
30	assign (segid 3A4 and resid 160 and name CB) (segid 3A4 and resid 430 and name CA)	12.62	4.01	4.01
	assign (segid 3A4 and resid 160 and name CB) (segid 3A4 and resid 431 and name CA)	11.04	3.14	3.13
	assign (segid 3A4 and resid 160 and name CB) (segid 3A4 and resid 433 and name CA)	13.97	2.01	2.02
	assign (segid 3A4 and resid 160 and name CB) (segid 3A4 and resid 436 and name CA)	16.27	1.07	1.07
	assign (segid 3A4 and resid 160 and name N) (segid 3A4 and resid 160 and name C)	2.48	0.02	0.02
35	assign (segid 3A4 and resid 160 and name N) (segid 3A4 and resid 160 and name CA)	1.46	0.00	0.01
	assign (segid 3A4 and resid 160 and name N) (segid 3A4 and resid 160 and name CB)	2.46	0.02	0.03
	assign (segid 3A4 and resid 160 and name N) (segid 3A4 and resid 160 and name O)	3.55	0.05	0.04
	assign (segid 3A4 and resid 160 and name N) (segid 3A4 and resid 161 and name C)	4.83	0.07	0.06
	assign (segid 3A4 and resid 160 and name N) (segid 3A4 and resid 161 and name CA)	4.25	0.06	0.05
40	assign (segid 3A4 and resid 160 and name N) (segid 3A4 and resid 161 and name CB)	5.07	0.11	0.10
	assign (segid 3A4 and resid 160 and name N) (segid 3A4 and resid 161 and name N)	2.82	0.05	0.06
	assign (segid 3A4 and resid 160 and name N) (segid 3A4 and resid 161 and name O)	5.98	0.09	0.09
	assign (segid 3A4 and resid 160 and name O) (segid 3A4 and resid 160 and name CB)	3.25	0.06	0.06
	assign (segid 3A4 and resid 160 and name O) (segid 3A4 and resid 161 and name C)	3.36	0.20	0.20
45	assign (segid 3A4 and resid 160 and name O) (segid 3A4 and resid 161 and name CA)	2.77	0.03	0.02
	assign (segid 3A4 and resid 160 and name O) (segid 3A4 and resid 161 and name CB)	4.16	0.06	0.05
	assign (segid 3A4 and resid 160 and name O) (segid 3A4 and resid 161 and name N)	2.25	0.01	0.01
	assign (segid 3A4 and resid 160 and name O) (segid 3A4 and resid 161 and name O)	4.11	0.35	0.35
50	assign (segid 3A4 and resid 161 and name C) (segid 3A4 and resid 161 and name CB)	2.50	0.04	0.04
	assign (segid 3A4 and resid 161 and name C) (segid 3A4 and resid 161 and name O)	1.23	0.01	0.01
	assign (segid 3A4 and resid 161 and name CA) (segid 3A4 and resid 161 and name C)	1.52	0.01	0.00
	assign (segid 3A4 and resid 161 and name CA) (segid 3A4 and resid 161 and name CB)	1.54	0.02	0.01
	assign (segid 3A4 and resid 161 and name CA) (segid 3A4 and resid 161 and name O)	2.39	0.02	0.02
	assign (segid 3A4 and resid 161 and name CA) (segid 3A4 and resid 187 and name CA)	9.61	1.13	1.13
55	assign (segid 3A4 and resid 161 and name CA) (segid 3A4 and resid 187 and name CB)	9.15	1.19	1.19
	assign (segid 3A4 and resid 161 and name CA) (segid 3A4 and resid 188 and name CA)	12.82	1.26	1.26
	assign (segid 3A4 and resid 161 and name CA) (segid 3A4 and resid 189 and name CA)	14.05	1.21	1.22
	assign (segid 3A4 and resid 161 and name CA) (segid 3A4 and resid 189 and name CB)	14.38	1.20	1.21
	assign (segid 3A4 and resid 161 and name CA) (segid 3A4 and resid 190 and name CA)	11.49	1.44	1.44
60	assign (segid 3A4 and resid 161 and name CA) (segid 3A4 and resid 190 and name CB)	10.11	1.43	1.43
	assign (segid 3A4 and resid 161 and name CA) (segid 3A4 and resid 191 and name CA)	11.88	1.68	1.69
	assign (segid 3A4 and resid 161 and name CA) (segid 3A4 and resid 191 and name CB)	11.80	1.64	1.63
	assign (segid 3A4 and resid 161 and name CA) (segid 3A4 and resid 192 and name CA)	15.54	1.61	1.61
	assign (segid 3A4 and resid 161 and name CA) (segid 3A4 and resid 192 and name CB)	16.27	1.41	1.42
65	assign (segid 3A4 and resid 161 and name CA) (segid 3A4 and resid 193 and name CB)	15.03	1.68	1.69
	assign (segid 3A4 and resid 161 and name CA) (segid 3A4 and resid 194 and name CA)	14.37	2.00	2.01
	assign (segid 3A4 and resid 161 and name CA) (segid 3A4 and resid 194 and name CB)	13.05	2.06	2.06
	assign (segid 3A4 and resid 161 and name CA) (segid 3A4 and resid 249 and name CA)	14.43	2.43	2.42
	assign (segid 3A4 and resid 161 and name CA) (segid 3A4 and resid 250 and name CA)	13.92	2.21	2.22
70	assign (segid 3A4 and resid 161 and name CA) (segid 3A4 and resid 250 and name CB)	14.79	2.16	2.16
	assign (segid 3A4 and resid 161 and name CA) (segid 3A4 and resid 252 and name CA)	13.87	2.31	2.32
	assign (segid 3A4 and resid 161 and name CA) (segid 3A4 and resid 252 and name CB)	13.84	2.34	2.34
	assign (segid 3A4 and resid 161 and name CA) (segid 3A4 and resid 253 and name CA)	10.45	2.24	2.24
	assign (segid 3A4 and resid 161 and name CA) (segid 3A4 and resid 254 and name CA)	12.12	2.07	2.07
75	assign (segid 3A4 and resid 161 and name CA) (segid 3A4 and resid 256 and name CA)	12.70	2.55	2.55
	assign (segid 3A4 and resid 161 and name CA) (segid 3A4 and resid 257 and name CA)	10.29	2.67	2.67
	assign (segid 3A4 and resid 161 and name CA) (segid 3A4 and resid 258 and name CA)	12.53	2.49	2.49
	assign (segid 3A4 and resid 161 and name CA) (segid 3A4 and resid 258 and name CB)	13.01	2.35	2.35
	assign (segid 3A4 and resid 161 and name CA) (segid 3A4 and resid 318 and name CA)	14.28	2.18	2.18
80	assign (segid 3A4 and resid 161 and name CA) (segid 3A4 and resid 318 and name CB)	14.15	2.29	2.28
	assign (segid 3A4 and resid 161 and name CA) (segid 3A4 and resid 319 and name CA)	13.35	2.14	2.14
	assign (segid 3A4 and resid 161 and name CA) (segid 3A4 and resid 319 and name CB)	13.66	2.04	2.05
	assign (segid 3A4 and resid 161 and name CA) (segid 3A4 and resid 427 and name CA)	13.09	2.20	2.20

	assign (segid 3A4 and resid 161 and name CA)	(segid 3A4 and resid 428 and name CA)	12.10	1.79	1.79
	assign (segid 3A4 and resid 161 and name CA)	(segid 3A4 and resid 429 and name CA)	10.54	2.67	2.66
	assign (segid 3A4 and resid 161 and name CA)	(segid 3A4 and resid 430 and name CA)	10.28	2.76	2.76
	assign (segid 3A4 and resid 161 and name CA)	(segid 3A4 and resid 431 and name CA)	9.26	2.20	2.19
5	assign (segid 3A4 and resid 161 and name CA)	(segid 3A4 and resid 433 and name CA)	11.76	2.22	2.22
	assign (segid 3A4 and resid 161 and name CA)	(segid 3A4 and resid 434 and name CA)	12.70	2.50	2.51
	assign (segid 3A4 and resid 161 and name CA)	(segid 3A4 and resid 436 and name CA)	14.21	2.17	2.17
	assign (segid 3A4 and resid 161 and name CB)	(segid 3A4 and resid 187 and name CA)	10.26	0.66	0.67
	assign (segid 3A4 and resid 161 and name CB)	(segid 3A4 and resid 187 and name CB)	9.88	0.82	0.83
10	assign (segid 3A4 and resid 161 and name CB)	(segid 3A4 and resid 188 and name CA)	13.40	0.82	0.81
	assign (segid 3A4 and resid 161 and name CB)	(segid 3A4 and resid 189 and name CA)	14.47	0.67	0.67
	assign (segid 3A4 and resid 161 and name CB)	(segid 3A4 and resid 189 and name CB)	14.78	0.69	0.69
	assign (segid 3A4 and resid 161 and name CB)	(segid 3A4 and resid 190 and name CA)	11.80	1.01	1.01
	assign (segid 3A4 and resid 161 and name CB)	(segid 3A4 and resid 190 and name CB)	10.44	0.99	0.99
15	assign (segid 3A4 and resid 161 and name CB)	(segid 3A4 and resid 191 and name CA)	12.21	1.48	1.48
	assign (segid 3A4 and resid 161 and name CB)	(segid 3A4 and resid 191 and name CB)	12.19	1.47	1.47
	assign (segid 3A4 and resid 161 and name CB)	(segid 3A4 and resid 192 and name CA)	15.80	1.36	1.35
	assign (segid 3A4 and resid 161 and name CB)	(segid 3A4 and resid 192 and name CB)	16.57	1.10	1.11
	assign (segid 3A4 and resid 161 and name CB)	(segid 3A4 and resid 193 and name CA)	15.77	1.47	1.48
20	assign (segid 3A4 and resid 161 and name CB)	(segid 3A4 and resid 193 and name CB)	15.14	1.37	1.36
	assign (segid 3A4 and resid 161 and name CB)	(segid 3A4 and resid 194 and name CA)	14.36	1.94	1.94
	assign (segid 3A4 and resid 161 and name CB)	(segid 3A4 and resid 194 and name CB)	13.04	2.04	2.04
	assign (segid 3A4 and resid 161 and name CB)	(segid 3A4 and resid 249 and name CA)	14.24	2.87	2.86
	assign (segid 3A4 and resid 161 and name CB)	(segid 3A4 and resid 250 and name CA)	13.72	2.71	2.70
25	assign (segid 3A4 and resid 161 and name CB)	(segid 3A4 and resid 252 and name CA)	13.40	2.76	2.76
	assign (segid 3A4 and resid 161 and name CB)	(segid 3A4 and resid 252 and name CB)	13.41	2.73	2.73
	assign (segid 3A4 and resid 161 and name CB)	(segid 3A4 and resid 253 and name CA)	10.03	2.73	2.72
	assign (segid 3A4 and resid 161 and name CB)	(segid 3A4 and resid 254 and name CA)	11.69	2.61	2.61
	assign (segid 3A4 and resid 161 and name CB)	(segid 3A4 and resid 256 and name CA)	12.01	3.01	3.01
30	assign (segid 3A4 and resid 161 and name CB)	(segid 3A4 and resid 257 and name CA)	9.62	3.18	3.18
	assign (segid 3A4 and resid 161 and name CB)	(segid 3A4 and resid 258 and name CA)	11.91	3.07	3.07
	assign (segid 3A4 and resid 161 and name CB)	(segid 3A4 and resid 258 and name CB)	12.44	2.95	2.95
	assign (segid 3A4 and resid 161 and name CB)	(segid 3A4 and resid 318 and name CA)	13.95	2.67	2.67
	assign (segid 3A4 and resid 161 and name CB)	(segid 3A4 and resid 319 and name CA)	13.21	2.56	2.57
35	assign (segid 3A4 and resid 161 and name CB)	(segid 3A4 and resid 319 and name CB)	13.49	2.50	2.51
	assign (segid 3A4 and resid 161 and name CB)	(segid 3A4 and resid 427 and name CA)	12.99	2.58	2.57
	assign (segid 3A4 and resid 161 and name CB)	(segid 3A4 and resid 428 and name CA)	12.26	2.03	2.04
	assign (segid 3A4 and resid 161 and name CB)	(segid 3A4 and resid 429 and name CA)	10.79	2.66	2.66
	assign (segid 3A4 and resid 161 and name CB)	(segid 3A4 and resid 430 and name CA)	10.69	2.60	2.60
40	assign (segid 3A4 and resid 161 and name CB)	(segid 3A4 and resid 431 and name CA)	9.62	2.20	2.20
	assign (segid 3A4 and resid 161 and name CB)	(segid 3A4 and resid 433 and name CA)	11.54	2.57	2.57
	assign (segid 3A4 and resid 161 and name CB)	(segid 3A4 and resid 434 and name CA)	12.23	2.93	2.94
	assign (segid 3A4 and resid 161 and name CB)	(segid 3A4 and resid 436 and name CA)	13.78	2.47	2.46
	assign (segid 3A4 and resid 161 and name N)	(segid 3A4 and resid 161 and name C)	2.48	0.03	0.04
45	assign (segid 3A4 and resid 161 and name N)	(segid 3A4 and resid 161 and name CA)	1.46	0.01	0.01
	assign (segid 3A4 and resid 161 and name N)	(segid 3A4 and resid 161 and name CB)	2.46	0.01	0.01
	assign (segid 3A4 and resid 161 and name N)	(segid 3A4 and resid 161 and name O)	3.57	0.05	0.05
	assign (segid 3A4 and resid 161 and name O)	(segid 3A4 and resid 161 and name CB)	3.06	0.15	0.16
	assign (segid 3A4 and resid 187 and name C)	(segid 3A4 and resid 187 and name CB)	2.52	0.02	0.02
50	assign (segid 3A4 and resid 187 and name C)	(segid 3A4 and resid 187 and name O)	1.24	0.01	0.00
	assign (segid 3A4 and resid 187 and name C)	(segid 3A4 and resid 188 and name C)	3.03	0.07	0.08
	assign (segid 3A4 and resid 187 and name C)	(segid 3A4 and resid 188 and name CA)	2.46	0.02	0.01
	assign (segid 3A4 and resid 187 and name C)	(segid 3A4 and resid 188 and name N)	1.33	0.00	0.01
	assign (segid 3A4 and resid 187 and name C)	(segid 3A4 and resid 188 and name O)	3.91	0.09	0.09
55	assign (segid 3A4 and resid 187 and name C)	(segid 3A4 and resid 189 and name C)	4.47	0.13	0.13
	assign (segid 3A4 and resid 187 and name C)	(segid 3A4 and resid 189 and name CA)	4.40	0.12	0.12
	assign (segid 3A4 and resid 187 and name C)	(segid 3A4 and resid 189 and name CB)	5.15	0.20	0.20
	assign (segid 3A4 and resid 187 and name C)	(segid 3A4 and resid 189 and name N)	3.23	0.11	0.11
	assign (segid 3A4 and resid 187 and name C)	(segid 3A4 and resid 189 and name O)	5.52	0.20	0.20
60	assign (segid 3A4 and resid 187 and name C)	(segid 3A4 and resid 190 and name C)	4.83	0.13	0.13
	assign (segid 3A4 and resid 187 and name C)	(segid 3A4 and resid 190 and name CA)	4.52	0.07	0.07
	assign (segid 3A4 and resid 187 and name C)	(segid 3A4 and resid 190 and name CB)	4.35	0.06	0.05
	assign (segid 3A4 and resid 187 and name C)	(segid 3A4 and resid 190 and name N)	3.78	0.06	0.06
	assign (segid 3A4 and resid 187 and name C)	(segid 3A4 and resid 190 and name O)	6.05	0.14	0.13
65	assign (segid 3A4 and resid 187 and name C)	(segid 3A4 and resid 191 and name C)	6.03	0.22	0.23
	assign (segid 3A4 and resid 187 and name C)	(segid 3A4 and resid 191 and name CA)	4.94	0.21	0.22
	assign (segid 3A4 and resid 187 and name C)	(segid 3A4 and resid 191 and name CB)	4.52	0.21	0.21
	assign (segid 3A4 and resid 187 and name C)	(segid 3A4 and resid 191 and name N)	4.06	0.17	0.17
	assign (segid 3A4 and resid 187 and name C)	(segid 3A4 and resid 191 and name O)	7.20	0.22	0.22
70	assign (segid 3A4 and resid 187 and name C)	(segid 3A4 and resid 192 and name CA)	7.20	0.30	0.29
	assign (segid 3A4 and resid 187 and name C)	(segid 3A4 and resid 192 and name CB)	7.21	0.34	0.34
	assign (segid 3A4 and resid 187 and name C)	(segid 3A4 and resid 192 and name N)	5.91	0.27	0.28
	assign (segid 3A4 and resid 187 and name CA)	(segid 3A4 and resid 187 and name C)	1.53	0.01	0.00
	assign (segid 3A4 and resid 187 and name CA)	(segid 3A4 and resid 187 and name CB)	1.53	0.01	0.02
75	assign (segid 3A4 and resid 187 and name CA)	(segid 3A4 and resid 187 and name O)	2.41	0.02	0.02
	assign (segid 3A4 and resid 187 and name CA)	(segid 3A4 and resid 188 and name C)	4.44	0.06	0.05
	assign (segid 3A4 and resid 187 and name CA)	(segid 3A4 and resid 188 and name CA)	3.81	0.02	0.03
	assign (segid 3A4 and resid 187 and name CA)	(segid 3A4 and resid 188 and name N)	2.42	0.02	0.02
	assign (segid 3A4 and resid 187 and name CA)	(segid 3A4 and resid 188 and name O)	5.39	0.08	0.07
80	assign (segid 3A4 and resid 187 and name CA)	(segid 3A4 and resid 189 and name C)	5.47	0.11	0.10
	assign (segid 3A4 and resid 187 and name CA)	(segid 3A4 and resid 189 and name CA)	5.43	0.12	0.12
	assign (segid 3A4 and resid 187 and name CA)	(segid 3A4 and resid 189 and name CB)	5.85	0.26	0.26
	assign (segid 3A4 and resid 187 and name CA)	(segid 3A4 and resid 189 and name N)	4.36	0.10	0.10

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5	assign	(segid 3A4 and resid 187 and name N)	(segid 3A4 and resid 187 and name CA)	1.46	0.01	0.00
	assign	(segid 3A4 and resid 187 and name N)	(segid 3A4 and resid 187 and name CB)	2.45	0.03	0.04
	assign	(segid 3A4 and resid 187 and name N)	(segid 3A4 and resid 187 and name O)	3.44	0.05	0.04
	assign	(segid 3A4 and resid 187 and name N)	(segid 3A4 and resid 188 and name C)	4.70	0.07	0.06
	assign	(segid 3A4 and resid 187 and name N)	(segid 3A4 and resid 188 and name CA)	4.19	0.04	0.05
10	assign	(segid 3A4 and resid 187 and name N)	(segid 3A4 and resid 188 and name N)	2.80	0.05	0.05
	assign	(segid 3A4 and resid 187 and name N)	(segid 3A4 and resid 188 and name O)	5.81	0.07	0.07
	assign	(segid 3A4 and resid 187 and name N)	(segid 3A4 and resid 189 and name C)	5.57	0.08	0.08
	assign	(segid 3A4 and resid 187 and name N)	(segid 3A4 and resid 189 and name CA)	5.27	0.15	0.15
	assign	(segid 3A4 and resid 187 and name N)	(segid 3A4 and resid 189 and name CB)	5.33	0.29	0.30
15	assign	(segid 3A4 and resid 187 and name N)	(segid 3A4 and resid 189 and name N)	4.26	0.11	0.12
	assign	(segid 3A4 and resid 187 and name N)	(segid 3A4 and resid 189 and name O)	6.77	0.10	0.10
	assign	(segid 3A4 and resid 187 and name N)	(segid 3A4 and resid 190 and name C)	6.43	0.11	0.11
	assign	(segid 3A4 and resid 187 and name N)	(segid 3A4 and resid 190 and name CA)	5.60	0.06	0.06
	assign	(segid 3A4 and resid 187 and name N)	(segid 3A4 and resid 190 and name CB)	5.07	0.06	0.06
20	assign	(segid 3A4 and resid 187 and name N)	(segid 3A4 and resid 190 and name N)	4.79	0.05	0.05
	assign	(segid 3A4 and resid 187 and name N)	(segid 3A4 and resid 190 and name O)	7.64	0.09	0.10
	assign	(segid 3A4 and resid 187 and name N)	(segid 3A4 and resid 191 and name CA)	7.13	0.21	0.20
	assign	(segid 3A4 and resid 187 and name N)	(segid 3A4 and resid 191 and name CB)	6.88	0.22	0.23
	assign	(segid 3A4 and resid 187 and name N)	(segid 3A4 and resid 191 and name N)	6.02	0.17	0.16
25	assign	(segid 3A4 and resid 187 and name O)	(segid 3A4 and resid 187 and name CB)	3.38	0.06	0.06
	assign	(segid 3A4 and resid 187 and name O)	(segid 3A4 and resid 188 and name C)	2.98	0.14	0.13
	assign	(segid 3A4 and resid 187 and name O)	(segid 3A4 and resid 188 and name CA)	2.82	0.03	0.04
	assign	(segid 3A4 and resid 187 and name O)	(segid 3A4 and resid 188 and name N)	2.27	0.03	0.02
	assign	(segid 3A4 and resid 187 and name O)	(segid 3A4 and resid 188 and name O)	3.51	0.15	0.15
30	assign	(segid 3A4 and resid 187 and name O)	(segid 3A4 and resid 189 and name C)	3.94	0.27	0.26
	assign	(segid 3A4 and resid 187 and name O)	(segid 3A4 and resid 189 and name CA)	4.24	0.23	0.24
	assign	(segid 3A4 and resid 187 and name O)	(segid 3A4 and resid 189 and name CB)	5.20	0.29	0.28
	assign	(segid 3A4 and resid 187 and name O)	(segid 3A4 and resid 189 and name N)	3.32	0.19	0.20
	assign	(segid 3A4 and resid 187 and name O)	(segid 3A4 and resid 189 and name O)	4.85	0.33	0.32
35	assign	(segid 3A4 and resid 187 and name O)	(segid 3A4 and resid 190 and name C)	3.73	0.17	0.18
	assign	(segid 3A4 and resid 187 and name O)	(segid 3A4 and resid 190 and name CA)	3.66	0.15	0.15
	assign	(segid 3A4 and resid 187 and name O)	(segid 3A4 and resid 190 and name CB)	3.60	0.05	0.04
	assign	(segid 3A4 and resid 187 and name O)	(segid 3A4 and resid 190 and name N)	3.17	0.17	0.17
	assign	(segid 3A4 and resid 187 and name O)	(segid 3A4 and resid 190 and name O)	4.92	0.17	0.18
40	assign	(segid 3A4 and resid 187 and name O)	(segid 3A4 and resid 191 and name C)	4.94	0.24	0.24
	assign	(segid 3A4 and resid 187 and name O)	(segid 3A4 and resid 191 and name CA)	3.79	0.20	0.19
	assign	(segid 3A4 and resid 187 and name O)	(segid 3A4 and resid 191 and name CB)	3.53	0.16	0.15
	assign	(segid 3A4 and resid 187 and name O)	(segid 3A4 and resid 191 and name N)	2.89	0.19	0.20
	assign	(segid 3A4 and resid 187 and name O)	(segid 3A4 and resid 191 and name O)	6.07	0.22	0.23
45	assign	(segid 3A4 and resid 187 and name O)	(segid 3A4 and resid 192 and name C)	7.18	0.31	0.31
	assign	(segid 3A4 and resid 187 and name O)	(segid 3A4 and resid 192 and name CA)	6.31	0.34	0.35
	assign	(segid 3A4 and resid 187 and name O)	(segid 3A4 and resid 192 and name CB)	6.52	0.41	0.40
	assign	(segid 3A4 and resid 187 and name O)	(segid 3A4 and resid 192 and name N)	4.96	0.32	0.32
	assign	(segid 3A4 and resid 187 and name O)	(segid 3A4 and resid 192 and name O)	6.83	0.27	0.27
50	assign	(segid 3A4 and resid 188 and name C)	(segid 3A4 and resid 188 and name O)	1.23	0.00	0.01
	assign	(segid 3A4 and resid 188 and name C)	(segid 3A4 and resid 189 and name C)	3.05	0.06	0.06
	assign	(segid 3A4 and resid 188 and name C)	(segid 3A4 and resid 189 and name CA)	2.43	0.03	0.04
	assign	(segid 3A4 and resid 188 and name C)	(segid 3A4 and resid 189 and name CB)	3.70	0.04	0.05
	assign	(segid 3A4 and resid 188 and name C)	(segid 3A4 and resid 189 and name N)	1.33	0.01	0.00
55	assign	(segid 3A4 and resid 188 and name C)	(segid 3A4 and resid 189 and name O)	3.85	0.17	0.17
	assign	(segid 3A4 and resid 188 and name C)	(segid 3A4 and resid 190 and name C)	4.64	0.10	0.10
	assign	(segid 3A4 and resid 188 and name C)	(segid 3A4 and resid 190 and name CA)	4.58	0.06	0.06
	assign	(segid 3A4 and resid 188 and name C)	(segid 3A4 and resid 190 and name CB)	5.35	0.09	0.09
	assign	(segid 3A4 and resid 188 and name C)	(segid 3A4 and resid 190 and name N)	3.40	0.07	0.06
60	assign	(segid 3A4 and resid 188 and name C)	(segid 3A4 and resid 190 and name O)	5.68	0.11	0.12
	assign	(segid 3A4 and resid 188 and name C)	(segid 3A4 and resid 191 and name C)	4.92	0.13	0.13
	assign	(segid 3A4 and resid 188 and name C)	(segid 3A4 and resid 191 and name CA)	4.59	0.18	0.18
	assign	(segid 3A4 and resid 188 and name C)	(segid 3A4 and resid 191 and name CB)	4.33	0.24	0.23
	assign	(segid 3A4 and resid 188 and name C)	(segid 3A4 and resid 191 and name N)	3.92	0.14	0.14
65	assign	(segid 3A4 and resid 188 and name C)	(segid 3A4 and resid 191 and name O)	6.13	0.13	0.12
	assign	(segid 3A4 and resid 188 and name C)	(segid 3A4 and resid 192 and name C)	6.18	0.15	0.16
	assign	(segid 3A4 and resid 188 and name C)	(segid 3A4 and resid 192 and name CA)	5.07	0.19	0.19
	assign	(segid 3A4 and resid 188 and name C)	(segid 3A4 and resid 192 and name CB)	4.62	0.27	0.26
	assign	(segid 3A4 and resid 188 and name C)	(segid 3A4 and resid 192 and name N)	4.18	0.14	0.14
70	assign	(segid 3A4 and resid 188 and name C)	(segid 3A4 and resid 192 and name O)	7.33	0.16	0.16
	assign	(segid 3A4 and resid 188 and name C)	(segid 3A4 and resid 193 and name CA)	7.39	0.17	0.17
	assign	(segid 3A4 and resid 188 and name C)	(segid 3A4 and resid 193 and name CB)	7.43	0.22	0.23
	assign	(segid 3A4 and resid 188 and name C)	(segid 3A4 and resid 193 and name N)	6.10	0.15	0.16
	assign	(segid 3A4 and resid 188 and name C)	(segid 3A4 and resid 193 and name O)	1.52	0.01	0.01
75	assign	(segid 3A4 and resid 188 and name CA)	(segid 3A4 and resid 188 and name C)	2.40	0.02	0.01
	assign	(segid 3A4 and resid 188 and name CA)	(segid 3A4 and resid 189 and name C)	4.42	0.05	0.04
	assign	(segid 3A4 and resid 188 and name CA)	(segid 3A4 and resid 189 and name CA)	3.80	0.02	0.02
	assign	(segid 3A4 and resid 188 and name CA)	(segid 3A4 and resid 189 and name CB)	4.86	0.02	0.01
	assign	(segid 3A4 and resid 188 and name CA)	(segid 3A4 and resid 189 and name N)	2.43	0.01	0.01
80	assign	(segid 3A4 and resid 188 and name CA)	(segid 3A4 and resid 189 and name O)	5.29	0.15	0.16
	assign	(segid 3A4 and resid 188 and name CA)	(segid 3A4 and resid 190 and name C)	5.56	0.09	0.08
	assign	(segid 3A4 and resid 188 and name CA)	(segid 3A4 and resid 190 and name CA)	5.53	0.06	0.07
	assign	(segid 3A4 and resid 188 and name CA)	(segid 3A4 and resid 190 and name CB)	5.97	0.10	0.10
	assign	(segid 3A4 and resid 188 and name CA)	(segid 3A4 and resid 190 and name N)	4.45	0.09	0.09
	assign	(segid 3A4 and resid 188 and name CA)	(segid 3A4 and resid 190 and name O)	6.66	0.10	0.11
	assign	(segid 3A4 and resid 188 and name CA)	(segid 3A4 and resid 191 and name C)	5.74	0.14	0.14
	assign	(segid 3A4 and resid 188 and name CA)	(segid 3A4 and resid 191 and name CA)	5.15	0.18	0.17

	assign (segid 3A4 and resid 188 and name CA)	(segid 3A4 and resid 191 and name CB)	4.46	0.22	0.23
	assign (segid 3A4 and resid 188 and name CA)	(segid 3A4 and resid 191 and name N)	4.62	0.12	0.12
	assign (segid 3A4 and resid 188 and name CA)	(segid 3A4 and resid 191 and name O)	6.93	0.15	0.14
	assign (segid 3A4 and resid 188 and name CA)	(segid 3A4 and resid 192 and name C)	7.44	0.18	0.18
	assign (segid 3A4 and resid 188 and name CA)	(segid 3A4 and resid 192 and name CA)	6.22	0.21	0.22
5	assign (segid 3A4 and resid 188 and name CA)	(segid 3A4 and resid 192 and name CB)	5.88	0.27	0.26
	assign (segid 3A4 and resid 188 and name CA)	(segid 3A4 and resid 192 and name N)	5.23	0.18	0.17
	assign (segid 3A4 and resid 188 and name CA)	(segid 3A4 and resid 192 and name CA)	8.74	0.16	0.17
	assign (segid 3A4 and resid 188 and name CA)	(segid 3A4 and resid 193 and name CB)	8.79	0.21	0.22
	assign (segid 3A4 and resid 188 and name CA)	(segid 3A4 and resid 193 and name N)	7.43	0.15	0.16
10	assign (segid 3A4 and resid 188 and name CA)	(segid 3A4 and resid 194 and name CA)	10.11	0.13	0.13
	assign (segid 3A4 and resid 188 and name CA)	(segid 3A4 and resid 194 and name CB)	9.76	0.15	0.16
	assign (segid 3A4 and resid 188 and name CA)	(segid 3A4 and resid 195 and name CA)	10.47	0.17	0.16
	assign (segid 3A4 and resid 188 and name CA)	(segid 3A4 and resid 195 and name CB)	9.61	0.19	0.19
	assign (segid 3A4 and resid 188 and name CA)	(segid 3A4 and resid 196 and name CA)	12.23	0.20	0.19
15	assign (segid 3A4 and resid 188 and name CA)	(segid 3A4 and resid 196 and name CB)	11.88	0.22	0.22
	assign (segid 3A4 and resid 188 and name CA)	(segid 3A4 and resid 197 and name CA)	14.39	0.33	0.33
	assign (segid 3A4 and resid 188 and name CA)	(segid 3A4 and resid 197 and name CB)	14.09	0.20	0.20
	assign (segid 3A4 and resid 188 and name CA)	(segid 3A4 and resid 198 and name CA)	15.47	0.16	0.15
	assign (segid 3A4 and resid 188 and name CA)	(segid 3A4 and resid 198 and name CB)	14.79	0.20	0.20
20	assign (segid 3A4 and resid 188 and name CA)	(segid 3A4 and resid 199 and name CA)	16.24	0.22	0.22
	assign (segid 3A4 and resid 188 and name CA)	(segid 3A4 and resid 199 and name CB)	15.40	0.30	0.30
	assign (segid 3A4 and resid 188 and name CA)	(segid 3A4 and resid 200 and name CA)	18.60	0.37	0.37
	assign (segid 3A4 and resid 188 and name CA)	(segid 3A4 and resid 242 and name CA)	16.68	1.57	1.57
	assign (segid 3A4 and resid 188 and name CA)	(segid 3A4 and resid 242 and name CB)	16.48	1.60	1.61
25	assign (segid 3A4 and resid 188 and name CA)	(segid 3A4 and resid 245 and name CA)	15.88	1.10	1.10
	assign (segid 3A4 and resid 188 and name CA)	(segid 3A4 and resid 245 and name CB)	15.02	1.23	1.23
	assign (segid 3A4 and resid 188 and name CA)	(segid 3A4 and resid 246 and name CA)	14.76	0.95	0.96
	assign (segid 3A4 and resid 188 and name CA)	(segid 3A4 and resid 246 and name CB)	14.88	1.04	1.04
	assign (segid 3A4 and resid 188 and name CA)	(segid 3A4 and resid 247 and name CA)	17.89	0.86	0.85
30	assign (segid 3A4 and resid 188 and name CA)	(segid 3A4 and resid 248 and name CA)	17.56	0.74	0.74
	assign (segid 3A4 and resid 188 and name CA)	(segid 3A4 and resid 248 and name CB)	17.58	0.73	0.73
	assign (segid 3A4 and resid 188 and name CA)	(segid 3A4 and resid 249 and name CA)	14.26	0.77	0.77
	assign (segid 3A4 and resid 188 and name CA)	(segid 3A4 and resid 250 and name CA)	15.93	0.89	0.89
	assign (segid 3A4 and resid 188 and name CA)	(segid 3A4 and resid 250 and name CB)	16.55	0.88	0.87
35	assign (segid 3A4 and resid 188 and name CA)	(segid 3A4 and resid 252 and name CA)	17.36	1.10	1.10
	assign (segid 3A4 and resid 188 and name CA)	(segid 3A4 and resid 252 and name CB)	16.40	1.09	1.10
	assign (segid 3A4 and resid 188 and name CA)	(segid 3A4 and resid 253 and name CA)	15.53	1.26	1.26
	assign (segid 3A4 and resid 188 and name N)	(segid 3A4 and resid 188 and name C)	2.47	0.02	0.02
40	assign (segid 3A4 and resid 188 and name N)	(segid 3A4 and resid 188 and name CA)	1.46	0.01	0.01
	assign (segid 3A4 and resid 188 and name N)	(segid 3A4 and resid 188 and name O)	3.52	0.03	0.03
	assign (segid 3A4 and resid 188 and name N)	(segid 3A4 and resid 189 and name C)	4.68	0.05	0.06
	assign (segid 3A4 and resid 188 and name N)	(segid 3A4 and resid 189 and name CA)	4.20	0.04	0.04
	assign (segid 3A4 and resid 188 and name N)	(segid 3A4 and resid 189 and name CB)	4.97	0.11	0.10
	assign (segid 3A4 and resid 188 and name N)	(segid 3A4 and resid 189 and name N)	2.80	0.04	0.05
45	assign (segid 3A4 and resid 188 and name N)	(segid 3A4 and resid 189 and name O)	5.74	0.13	0.14
	assign (segid 3A4 and resid 188 and name N)	(segid 3A4 and resid 190 and name C)	5.63	0.10	0.09
	assign (segid 3A4 and resid 188 and name N)	(segid 3A4 and resid 190 and name CA)	5.35	0.07	0.08
	assign (segid 3A4 and resid 188 and name N)	(segid 3A4 and resid 190 and name CB)	5.44	0.10	0.10
	assign (segid 3A4 and resid 188 and name N)	(segid 3A4 and resid 190 and name N)	4.34	0.08	0.09
50	assign (segid 3A4 and resid 188 and name N)	(segid 3A4 and resid 191 and name C)	6.83	0.11	0.11
	assign (segid 3A4 and resid 188 and name N)	(segid 3A4 and resid 191 and name CA)	6.42	0.18	0.18
	assign (segid 3A4 and resid 188 and name N)	(segid 3A4 and resid 191 and name CB)	5.54	0.18	0.18
	assign (segid 3A4 and resid 188 and name N)	(segid 3A4 and resid 191 and name N)	4.94	0.21	0.22
	assign (segid 3A4 and resid 188 and name N)	(segid 3A4 and resid 191 and name O)	4.79	0.13	0.13
55	assign (segid 3A4 and resid 188 and name N)	(segid 3A4 and resid 192 and name CA)	7.61	0.18	0.18
	assign (segid 3A4 and resid 188 and name N)	(segid 3A4 and resid 192 and name CB)	7.22	0.24	0.24
	assign (segid 3A4 and resid 188 and name N)	(segid 3A4 and resid 192 and name N)	7.00	0.28	0.28
	assign (segid 3A4 and resid 188 and name N)	(segid 3A4 and resid 192 and name O)	6.08	0.21	0.22
60	assign (segid 3A4 and resid 188 and name O)	(segid 3A4 and resid 189 and name C)	3.06	0.10	0.10
	assign (segid 3A4 and resid 188 and name O)	(segid 3A4 and resid 189 and name CA)	2.77	0.06	0.06
	assign (segid 3A4 and resid 188 and name O)	(segid 3A4 and resid 189 and name CB)	4.24	0.08	0.07
	assign (segid 3A4 and resid 188 and name O)	(segid 3A4 and resid 189 and name N)	2.25	0.01	0.01
	assign (segid 3A4 and resid 188 and name O)	(segid 3A4 and resid 189 and name O)	3.48	0.24	0.24
65	assign (segid 3A4 and resid 188 and name O)	(segid 3A4 and resid 190 and name C)	4.32	0.15	0.14
	assign (segid 3A4 and resid 188 and name O)	(segid 3A4 and resid 190 and name CA)	4.60	0.09	0.09
	assign (segid 3A4 and resid 188 and name O)	(segid 3A4 and resid 190 and name CB)	5.59	0.10	0.10
	assign (segid 3A4 and resid 188 and name O)	(segid 3A4 and resid 190 and name N)	3.62	0.07	0.08
	assign (segid 3A4 and resid 188 and name O)	(segid 3A4 and resid 190 and name O)	5.18	0.16	0.17
	assign (segid 3A4 and resid 188 and name O)	(segid 3A4 and resid 191 and name C)	3.97	0.15	0.15
70	assign (segid 3A4 and resid 188 and name O)	(segid 3A4 and resid 191 and name CA)	3.94	0.21	0.21
	assign (segid 3A4 and resid 188 and name O)	(segid 3A4 and resid 191 and name CB)	3.75	0.26	0.26
	assign (segid 3A4 and resid 188 and name O)	(segid 3A4 and resid 191 and name N)	3.55	0.17	0.17
	assign (segid 3A4 and resid 188 and name O)	(segid 3A4 and resid 191 and name O)	5.13	0.15	0.14
	assign (segid 3A4 and resid 188 and name O)	(segid 3A4 and resid 192 and name C)	5.12	0.19	0.20
75	assign (segid 3A4 and resid 188 and name O)	(segid 3A4 and resid 192 and name CA)	3.91	0.21	0.20
	assign (segid 3A4 and resid 188 and name O)	(segid 3A4 and resid 192 and name CB)	3.52	0.27	0.26
	assign (segid 3A4 and resid 188 and name O)	(segid 3A4 and resid 192 and name N)	3.11	0.17	0.16
	assign (segid 3A4 and resid 188 and name O)	(segid 3A4 and resid 192 and name O)	6.22	0.19	0.20
80	assign (segid 3A4 and resid 188 and name O)	(segid 3A4 and resid 193 and name C)	7.46	0.19	0.20
	assign (segid 3A4 and resid 188 and name O)	(segid 3A4 and resid 193 and name CA)	6.59	0.21	0.20
	assign (segid 3A4 and resid 188 and name O)	(segid 3A4 and resid 193 and name CB)	6.85	0.24	0.23
	assign (segid 3A4 and resid 188 and name O)	(segid 3A4 and resid 193 and name N)	5.21	0.20	0.20

	assign (segid 3A4 and resid 188 and name O) (segid 3A4 and resid 194 and name N)	7.19	0.19	0.18
	assign (segid 3A4 and resid 188 and name O) (segid 3A4 and resid 195 and name CB)	7.66	0.14	0.14
	assign (segid 3A4 and resid 189 and name C) (segid 3A4 and resid 189 and name CB)	2.49	0.05	0.05
	assign (segid 3A4 and resid 189 and name C) (segid 3A4 and resid 189 and name O)	1.23	0.00	0.00
5	assign (segid 3A4 and resid 189 and name C) (segid 3A4 and resid 190 and name C)	3.02	0.06	0.06
	assign (segid 3A4 and resid 189 and name C) (segid 3A4 and resid 190 and name CA)	2.44	0.01	0.01
	assign (segid 3A4 and resid 189 and name C) (segid 3A4 and resid 190 and name CB)	3.71	0.03	0.04
	assign (segid 3A4 and resid 189 and name C) (segid 3A4 and resid 190 and name N)	1.34	0.01	0.00
	assign (segid 3A4 and resid 189 and name C) (segid 3A4 and resid 190 and name O)	3.84	0.06	0.07
	assign (segid 3A4 and resid 189 and name C) (segid 3A4 and resid 191 and name C)	4.53	0.07	0.07
10	assign (segid 3A4 and resid 189 and name C) (segid 3A4 and resid 191 and name CA)	4.45	0.09	0.09
	assign (segid 3A4 and resid 189 and name C) (segid 3A4 and resid 191 and name CB)	5.18	0.13	0.13
	assign (segid 3A4 and resid 189 and name C) (segid 3A4 and resid 191 and name N)	3.29	0.10	0.10
	assign (segid 3A4 and resid 189 and name C) (segid 3A4 and resid 191 and name O)	5.59	0.06	0.06
15	assign (segid 3A4 and resid 189 and name C) (segid 3A4 and resid 192 and name C)	4.89	0.08	0.08
	assign (segid 3A4 and resid 189 and name C) (segid 3A4 and resid 192 and name CA)	4.50	0.14	0.15
	assign (segid 3A4 and resid 189 and name C) (segid 3A4 and resid 192 and name CB)	4.27	0.29	0.30
	assign (segid 3A4 and resid 189 and name C) (segid 3A4 and resid 192 and name N)	3.79	0.11	0.11
	assign (segid 3A4 and resid 189 and name C) (segid 3A4 and resid 192 and name O)	6.10	0.08	0.07
20	assign (segid 3A4 and resid 189 and name C) (segid 3A4 and resid 193 and name C)	6.25	0.10	0.11
	assign (segid 3A4 and resid 189 and name C) (segid 3A4 and resid 193 and name CA)	5.13	0.12	0.12
	assign (segid 3A4 and resid 189 and name C) (segid 3A4 and resid 193 and name CB)	4.75	0.21	0.22
	assign (segid 3A4 and resid 189 and name C) (segid 3A4 and resid 193 and name N)	4.21	0.08	0.07
	assign (segid 3A4 and resid 189 and name C) (segid 3A4 and resid 193 and name O)	7.40	0.11	0.11
25	assign (segid 3A4 and resid 189 and name C) (segid 3A4 and resid 194 and name CA)	7.47	0.11	0.11
	assign (segid 3A4 and resid 189 and name C) (segid 3A4 and resid 194 and name CB)	7.57	0.14	0.15
	assign (segid 3A4 and resid 189 and name C) (segid 3A4 and resid 194 and name N)	6.16	0.10	0.10
	assign (segid 3A4 and resid 189 and name C) (segid 3A4 and resid 195 and name N)	7.83	0.05	0.06
	assign (segid 3A4 and resid 189 and name CA) (segid 3A4 and resid 189 and name CB)	1.53	0.01	0.01
30	assign (segid 3A4 and resid 189 and name CA) (segid 3A4 and resid 189 and name O)	2.39	0.01	0.02
	assign (segid 3A4 and resid 189 and name CA) (segid 3A4 and resid 190 and name C)	4.42	0.04	0.03
	assign (segid 3A4 and resid 189 and name CA) (segid 3A4 and resid 190 and name CA)	3.82	0.02	0.03
	assign (segid 3A4 and resid 189 and name CA) (segid 3A4 and resid 190 and name CB)	4.88	0.07	0.06
35	assign (segid 3A4 and resid 189 and name CA) (segid 3A4 and resid 190 and name N)	2.45	0.03	0.03
	assign (segid 3A4 and resid 189 and name CA) (segid 3A4 and resid 190 and name O)	5.31	0.04	0.04
	assign (segid 3A4 and resid 189 and name CA) (segid 3A4 and resid 191 and name C)	5.49	0.06	0.06
	assign (segid 3A4 and resid 189 and name CA) (segid 3A4 and resid 191 and name CA)	5.44	0.08	0.09
	assign (segid 3A4 and resid 189 and name CA) (segid 3A4 and resid 191 and name CB)	5.82	0.13	0.14
40	assign (segid 3A4 and resid 189 and name CA) (segid 3A4 and resid 191 and name N)	4.39	0.08	0.09
	assign (segid 3A4 and resid 189 and name CA) (segid 3A4 and resid 191 and name O)	6.62	0.06	0.05
	assign (segid 3A4 and resid 189 and name CA) (segid 3A4 and resid 192 and name C)	5.76	0.09	0.08
	assign (segid 3A4 and resid 189 and name CA) (segid 3A4 and resid 192 and name CA)	5.12	0.15	0.16
	assign (segid 3A4 and resid 189 and name CA) (segid 3A4 and resid 192 and name CB)	4.48	0.31	0.31
45	assign (segid 3A4 and resid 189 and name CA) (segid 3A4 and resid 192 and name N)	4.56	0.09	0.09
	assign (segid 3A4 and resid 189 and name CA) (segid 3A4 and resid 192 and name O)	6.92	0.08	0.09
	assign (segid 3A4 and resid 189 and name CA) (segid 3A4 and resid 193 and name C)	7.53	0.10	0.10
	assign (segid 3A4 and resid 189 and name CA) (segid 3A4 and resid 193 and name CA)	6.31	0.11	0.12
	assign (segid 3A4 and resid 189 and name CA) (segid 3A4 and resid 193 and name CB)	6.04	0.21	0.20
50	assign (segid 3A4 and resid 189 and name CA) (segid 3A4 and resid 193 and name N)	5.30	0.07	0.07
	assign (segid 3A4 and resid 189 and name CA) (segid 3A4 and resid 194 and name CA)	8.84	0.09	0.09
	assign (segid 3A4 and resid 189 and name CA) (segid 3A4 and resid 194 and name CB)	8.97	0.14	0.14
	assign (segid 3A4 and resid 189 and name CA) (segid 3A4 and resid 194 and name N)	7.52	0.09	0.09
	assign (segid 3A4 and resid 189 and name CA) (segid 3A4 and resid 195 and name CA)	9.84	0.08	0.07
55	assign (segid 3A4 and resid 189 and name CA) (segid 3A4 and resid 195 and name CB)	9.34	0.09	0.09
	assign (segid 3A4 and resid 189 and name CA) (segid 3A4 and resid 196 and name CA)	10.54	0.13	0.13
	assign (segid 3A4 and resid 189 and name CA) (segid 3A4 and resid 196 and name CB)	9.81	0.17	0.18
	assign (segid 3A4 and resid 189 and name CA) (segid 3A4 and resid 197 and name CA)	12.49	0.11	0.10
	assign (segid 3A4 and resid 189 and name CA) (segid 3A4 and resid 197 and name CB)	12.14	0.11	0.11
60	assign (segid 3A4 and resid 189 and name CA) (segid 3A4 and resid 198 and name CA)	14.42	0.08	0.09
	assign (segid 3A4 and resid 189 and name CA) (segid 3A4 and resid 198 and name CB)	14.09	0.10	0.10
	assign (segid 3A4 and resid 189 and name CA) (segid 3A4 and resid 199 and name CA)	15.26	0.16	0.17
	assign (segid 3A4 and resid 189 and name CA) (segid 3A4 and resid 199 and name CB)	14.43	0.25	0.25
	assign (segid 3A4 and resid 189 and name CA) (segid 3A4 and resid 200 and name CA)	16.98	0.43	0.42
65	assign (segid 3A4 and resid 189 and name CA) (segid 3A4 and resid 201 and name CA)	18.89	0.32	0.31
	assign (segid 3A4 and resid 189 and name CA) (segid 3A4 and resid 201 and name CB)	18.47	0.38	0.38
	assign (segid 3A4 and resid 189 and name CA) (segid 3A4 and resid 202 and name CB)	19.28	0.25	0.24
	assign (segid 3A4 and resid 189 and name CA) (segid 3A4 and resid 245 and name CB)	16.29	0.93	0.94
	assign (segid 3A4 and resid 189 and name CA) (segid 3A4 and resid 246 and name CA)	15.37	1.09	1.09
70	assign (segid 3A4 and resid 189 and name CA) (segid 3A4 and resid 246 and name CB)	15.97	0.71	0.70
	assign (segid 3A4 and resid 189 and name CA) (segid 3A4 and resid 248 and name CA)	16.38	0.78	0.78
	assign (segid 3A4 and resid 189 and name CA) (segid 3A4 and resid 248 and name CB)	17.90	0.56	0.57
	assign (segid 3A4 and resid 189 and name CA) (segid 3A4 and resid 249 and name CA)	17.67	0.59	0.60
	assign (segid 3A4 and resid 189 and name CA) (segid 3A4 and resid 250 and name CA)	14.79	0.62	0.62
75	assign (segid 3A4 and resid 189 and name CA) (segid 3A4 and resid 250 and name CB)	17.10	0.76	0.75
	assign (segid 3A4 and resid 189 and name CA) (segid 3A4 and resid 252 and name CA)	17.94	0.71	0.72
	assign (segid 3A4 and resid 189 and name CA) (segid 3A4 and resid 252 and name CB)	17.50	1.03	1.02
	assign (segid 3A4 and resid 189 and name CA) (segid 3A4 and resid 253 and name CB)	16.33	1.02	1.02
	assign (segid 3A4 and resid 189 and name CA) (segid 3A4 and resid 253 and name CA)	16.17	1.15	1.16
80	assign (segid 3A4 and resid 189 and name CB) (segid 3A4 and resid 190 and name C)	5.39	0.14	0.15
	assign (segid 3A4 and resid 189 and name CB) (segid 3A4 and resid 190 and name CA)	1.44	0.16	0.17
	assign (segid 3A4 and resid 189 and name CB) (segid 3A4 and resid 190 and name CB)	5.30	0.23	0.24
	assign (segid 3A4 and resid 189 and name CB) (segid 3A4 and resid 190 and name N)	3.12	0.17	0.18

	assign (segid 3A4 and resid 189 and name CB)	(segid 3A4 and resid 190 and name O)	6.25	0.13	0.13
	assign (segid 3A4 and resid 189 and name CB)	(segid 3A4 and resid 191 and name C)	6.87	0.07	0.07
	assign (segid 3A4 and resid 189 and name CB)	(segid 3A4 and resid 191 and name CA)	6.77	0.13	0.13
	assign (segid 3A4 and resid 189 and name CB)	(segid 3A4 and resid 191 and name CB)	7.23	0.18	0.17
5	assign (segid 3A4 and resid 189 and name CB)	(segid 3A4 and resid 191 and name N)	5.59	0.16	0.16
	assign (segid 3A4 and resid 189 and name CB)	(segid 3A4 and resid 192 and name C)	6.88	0.12	0.12
	assign (segid 3A4 and resid 189 and name CB)	(segid 3A4 and resid 192 and name CA)	6.44	0.19	0.19
	assign (segid 3A4 and resid 189 and name CB)	(segid 3A4 and resid 192 and name CB)	5.72	0.36	0.36
	assign (segid 3A4 and resid 189 and name CB)	(segid 3A4 and resid 192 and name N)	5.97	0.11	0.10
10	assign (segid 3A4 and resid 189 and name CB)	(segid 3A4 and resid 193 and name CA)	7.06	0.22	0.12
	assign (segid 3A4 and resid 189 and name CB)	(segid 3A4 and resid 193 and name CB)	6.53	0.21	0.21
	assign (segid 3A4 and resid 189 and name CB)	(segid 3A4 and resid 193 and name N)	6.27	0.08	0.07
	assign (segid 3A4 and resid 189 and name CB)	(segid 3A4 and resid 194 and name CA)	9.83	0.13	0.13
	assign (segid 3A4 and resid 189 and name CB)	(segid 3A4 and resid 194 and name CB)	10.01	0.18	0.17
15	assign (segid 3A4 and resid 189 and name CB)	(segid 3A4 and resid 195 and name CA)	11.09	0.11	0.10
	assign (segid 3A4 and resid 189 and name CB)	(segid 3A4 and resid 195 and name CB)	10.68	0.10	0.11
	assign (segid 3A4 and resid 189 and name CB)	(segid 3A4 and resid 196 and name CA)	11.49	0.17	0.18
	assign (segid 3A4 and resid 189 and name CB)	(segid 3A4 and resid 196 and name CB)	10.63	0.20	0.21
	assign (segid 3A4 and resid 189 and name CB)	(segid 3A4 and resid 197 and name CA)	13.28	0.11	0.11
20	assign (segid 3A4 and resid 189 and name CB)	(segid 3A4 and resid 197 and name CB)	12.88	0.12	0.12
	assign (segid 3A4 and resid 189 and name CB)	(segid 3A4 and resid 198 and name CA)	15.48	0.09	0.09
	assign (segid 3A4 and resid 189 and name CB)	(segid 3A4 and resid 198 and name CB)	15.23	0.12	0.12
	assign (segid 3A4 and resid 189 and name CB)	(segid 3A4 and resid 199 and name CA)	16.37	0.19	0.20
	assign (segid 3A4 and resid 189 and name CB)	(segid 3A4 and resid 199 and name CB)	15.55	0.30	0.29
25	assign (segid 3A4 and resid 189 and name CB)	(segid 3A4 and resid 200 and name CA)	17.86	0.43	0.43
	assign (segid 3A4 and resid 189 and name CB)	(segid 3A4 and resid 245 and name CA)	17.66	0.92	0.93
	assign (segid 3A4 and resid 189 and name CB)	(segid 3A4 and resid 245 and name CB)	16.75	1.08	1.07
	assign (segid 3A4 and resid 189 and name CB)	(segid 3A4 and resid 246 and name CA)	17.39	0.71	0.72
	assign (segid 3A4 and resid 189 and name CB)	(segid 3A4 and resid 246 and name CB)	17.84	0.79	0.79
30	assign (segid 3A4 and resid 189 and name CB)	(segid 3A4 and resid 249 and name CA)	16.02	0.69	0.69
	assign (segid 3A4 and resid 189 and name CB)	(segid 3A4 and resid 250 and name CA)	18.32	0.87	0.86
	assign (segid 3A4 and resid 189 and name CB)	(segid 3A4 and resid 252 and name CB)	17.30	1.13	1.12
	assign (segid 3A4 and resid 189 and name N)	(segid 3A4 and resid 189 and name C)	2.44	0.01	0.02
35	assign (segid 3A4 and resid 189 and name N)	(segid 3A4 and resid 189 and name CA)	1.46	0.01	0.00
	assign (segid 3A4 and resid 189 and name N)	(segid 3A4 and resid 189 and name CB)	2.46	0.02	0.02
	assign (segid 3A4 and resid 189 and name N)	(segid 3A4 and resid 189 and name O)	3.47	0.07	0.07
	assign (segid 3A4 and resid 189 and name N)	(segid 3A4 and resid 190 and name C)	4.70	0.06	0.07
	assign (segid 3A4 and resid 189 and name N)	(segid 3A4 and resid 190 and name CA)	4.23	0.03	0.03
	assign (segid 3A4 and resid 189 and name N)	(segid 3A4 and resid 190 and name CB)	4.99	0.07	0.06
40	assign (segid 3A4 and resid 189 and name N)	(segid 3A4 and resid 190 and name N)	2.83	0.04	0.04
	assign (segid 3A4 and resid 189 and name N)	(segid 3A4 and resid 191 and name C)	5.77	0.07	0.07
	assign (segid 3A4 and resid 189 and name N)	(segid 3A4 and resid 191 and name CA)	5.61	0.09	0.09
	assign (segid 3A4 and resid 189 and name N)	(segid 3A4 and resid 191 and name CB)	5.29	0.15	0.14
	assign (segid 3A4 and resid 189 and name N)	(segid 3A4 and resid 191 and name N)	5.30	0.20	0.21
45	assign (segid 3A4 and resid 189 and name N)	(segid 3A4 and resid 191 and name O)	4.31	0.12	0.12
	assign (segid 3A4 and resid 189 and name N)	(segid 3A4 and resid 192 and name C)	6.82	0.09	0.08
	assign (segid 3A4 and resid 189 and name N)	(segid 3A4 and resid 192 and name CA)	6.51	0.10	0.10
	assign (segid 3A4 and resid 189 and name N)	(segid 3A4 and resid 192 and name CB)	5.61	0.15	0.16
	assign (segid 3A4 and resid 189 and name N)	(segid 3A4 and resid 192 and name N)	5.05	0.27	0.27
50	assign (segid 3A4 and resid 189 and name N)	(segid 3A4 and resid 192 and name O)	4.82	0.11	0.10
	assign (segid 3A4 and resid 189 and name N)	(segid 3A4 and resid 193 and name CA)	7.69	0.10	0.10
	assign (segid 3A4 and resid 189 and name N)	(segid 3A4 and resid 193 and name CB)	7.34	0.13	0.13
	assign (segid 3A4 and resid 189 and name N)	(segid 3A4 and resid 193 and name N)	7.15	0.21	0.21
	assign (segid 3A4 and resid 189 and name N)	(segid 3A4 and resid 193 and name O)	6.20	0.10	0.09
55	assign (segid 3A4 and resid 189 and name O)	(segid 3A4 and resid 189 and name CB)	3.28	0.10	0.09
	assign (segid 3A4 and resid 189 and name O)	(segid 3A4 and resid 190 and name C)	2.98	0.07	0.08
	assign (segid 3A4 and resid 189 and name O)	(segid 3A4 and resid 190 and name CA)	2.78	0.02	0.02
	assign (segid 3A4 and resid 189 and name O)	(segid 3A4 and resid 190 and name CB)	4.26	0.04	0.03
	assign (segid 3A4 and resid 189 and name O)	(segid 3A4 and resid 190 and name N)	2.25	0.01	0.01
60	assign (segid 3A4 and resid 189 and name O)	(segid 3A4 and resid 190 and name O)	3.43	0.09	0.09
	assign (segid 3A4 and resid 189 and name O)	(segid 3A4 and resid 191 and name C)	4.11	0.16	0.15
	assign (segid 3A4 and resid 189 and name O)	(segid 3A4 and resid 191 and name CA)	4.40	0.12	0.13
	assign (segid 3A4 and resid 189 and name O)	(segid 3A4 and resid 191 and name CB)	5.34	0.19	0.20
	assign (segid 3A4 and resid 189 and name O)	(segid 3A4 and resid 191 and name N)	3.47	0.11	0.11
65	assign (segid 3A4 and resid 189 and name O)	(segid 3A4 and resid 191 and name O)	5.01	0.14	0.14
	assign (segid 3A4 and resid 189 and name O)	(segid 3A4 and resid 192 and name C)	3.84	0.14	0.14
	assign (segid 3A4 and resid 189 and name O)	(segid 3A4 and resid 192 and name CA)	3.71	0.23	0.23
	assign (segid 3A4 and resid 189 and name O)	(segid 3A4 and resid 192 and name CB)	3.56	0.36	0.36
	assign (segid 3A4 and resid 189 and name O)	(segid 3A4 and resid 192 and name N)	3.28	0.21	0.20
70	assign (segid 3A4 and resid 189 and name O)	(segid 3A4 and resid 192 and name O)	5.02	0.13	0.12
	assign (segid 3A4 and resid 189 and name O)	(segid 3A4 and resid 193 and name C)	5.19	0.10	0.10
	assign (segid 3A4 and resid 189 and name O)	(segid 3A4 and resid 193 and name CA)	3.98	0.12	0.12
	assign (segid 3A4 and resid 189 and name O)	(segid 3A4 and resid 193 and name CB)	3.73	0.25	0.25
	assign (segid 3A4 and resid 189 and name O)	(segid 3A4 and resid 193 and name N)	3.09	0.08	0.07
75	assign (segid 3A4 and resid 189 and name O)	(segid 3A4 and resid 193 and name O)	6.30	0.11	0.10
	assign (segid 3A4 and resid 189 and name O)	(segid 3A4 and resid 194 and name C)	7.37	0.10	0.10
	assign (segid 3A4 and resid 189 and name O)	(segid 3A4 and resid 194 and name CA)	6.63	0.10	0.11
	assign (segid 3A4 and resid 189 and name O)	(segid 3A4 and resid 194 and name CB)	6.94	0.15	0.15
	assign (segid 3A4 and resid 189 and name O)	(segid 3A4 and resid 194 and name N)	5.26	0.10	0.09
80	assign (segid 3A4 and resid 189 and name O)	(segid 3A4 and resid 195 and name CB)	7.72	0.15	0.16
	assign (segid 3A4 and resid 189 and name O)	(segid 3A4 and resid 195 and name N)	6.96	0.07	0.07
	assign (segid 3A4 and resid 189 and name O)	(segid 3A4 and resid 196 and name N)	7.73	0.08	0.09
	assign (segid 3A4 and resid 190 and name C)	(segid 3A4 and resid 190 and name CB)	2.50	0.02	0.02

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	assign (segid 3A4 and resid 190 and name CB)	(segid 3A4 and resid 191 and name C)	5.39	0.08	0.07
	assign (segid 3A4 and resid 190 and name CB)	(segid 3A4 and resid 191 and name CA)	4.46	0.04	0.03
	assign (segid 3A4 and resid 190 and name CB)	(segid 3A4 and resid 191 and name CB)	5.33	0.02	0.03
	assign (segid 3A4 and resid 190 and name CB)	(segid 3A4 and resid 191 and name N)	3.12	0.04	0.05
	assign (segid 3A4 and resid 190 and name CB)	(segid 3A4 and resid 191 and name O)	6.23	0.09	0.08
5	assign (segid 3A4 and resid 190 and name CB)	(segid 3A4 and resid 192 and name C)	6.88	0.12	0.12
	assign (segid 3A4 and resid 190 and name CB)	(segid 3A4 and resid 192 and name CA)	6.77	0.13	0.13
	assign (segid 3A4 and resid 190 and name CB)	(segid 3A4 and resid 192 and name CB)	7.23	0.23	0.24
	assign (segid 3A4 and resid 190 and name CB)	(segid 3A4 and resid 192 and name N)	5.59	0.11	0.11
	assign (segid 3A4 and resid 190 and name CB)	(segid 3A4 and resid 193 and name C)	6.91	0.08	0.08
10	assign (segid 3A4 and resid 190 and name CB)	(segid 3A4 and resid 193 and name CA)	6.42	0.11	0.11
	assign (segid 3A4 and resid 190 and name CB)	(segid 3A4 and resid 193 and name CB)	5.63	0.18	0.19
	assign (segid 3A4 and resid 190 and name CB)	(segid 3A4 and resid 193 and name N)	5.95	0.12	0.11
	assign (segid 3A4 and resid 190 and name CB)	(segid 3A4 and resid 194 and name CA)	7.14	0.10	0.10
	assign (segid 3A4 and resid 190 and name CB)	(segid 3A4 and resid 194 and name CB)	6.64	0.12	0.12
15	assign (segid 3A4 and resid 190 and name CB)	(segid 3A4 and resid 194 and name N)	6.27	0.08	0.09
	assign (segid 3A4 and resid 190 and name CB)	(segid 3A4 and resid 195 and name CA)	9.62	0.08	0.09
	assign (segid 3A4 and resid 190 and name CB)	(segid 3A4 and resid 195 and name CB)	9.64	0.10	0.11
	assign (segid 3A4 and resid 190 and name CB)	(segid 3A4 and resid 196 and name CA)	11.19	0.10	0.09
	assign (segid 3A4 and resid 190 and name CB)	(segid 3A4 and resid 196 and name CB)	10.84	0.12	0.11
20	assign (segid 3A4 and resid 190 and name CB)	(segid 3A4 and resid 197 and name CA)	11.79	0.16	0.15
	assign (segid 3A4 and resid 190 and name CB)	(segid 3A4 and resid 197 and name CB)	10.92	0.24	0.24
	assign (segid 3A4 and resid 190 and name CB)	(segid 3A4 and resid 198 and name CA)	13.38	0.13	0.13
	assign (segid 3A4 and resid 190 and name CB)	(segid 3A4 and resid 198 and name CB)	12.86	0.12	0.13
	assign (segid 3A4 and resid 190 and name CB)	(segid 3A4 and resid 199 and name CA)	15.36	0.10	0.09
25	assign (segid 3A4 and resid 190 and name CB)	(segid 3A4 and resid 199 and name CB)	14.96	0.16	0.16
	assign (segid 3A4 and resid 190 and name CB)	(segid 3A4 and resid 200 and name CA)	17.05	0.44	0.45
	assign (segid 3A4 and resid 190 and name CB)	(segid 3A4 and resid 201 and name CA)	18.04	0.43	0.44
	assign (segid 3A4 and resid 190 and name CB)	(segid 3A4 and resid 201 and name CB)	17.27	0.51	0.52
	assign (segid 3A4 and resid 190 and name CB)	(segid 3A4 and resid 202 and name CA)	19.47	0.19	0.20
30	assign (segid 3A4 and resid 190 and name CB)	(segid 3A4 and resid 202 and name CB)	18.83	0.21	0.22
	assign (segid 3A4 and resid 190 and name CB)	(segid 3A4 and resid 245 and name CA)	15.41	0.95	0.96
	assign (segid 3A4 and resid 190 and name CB)	(segid 3A4 and resid 245 and name CB)	14.88	1.12	1.13
	assign (segid 3A4 and resid 190 and name CB)	(segid 3A4 and resid 246 and name CA)	14.71	0.80	0.79
	assign (segid 3A4 and resid 190 and name CB)	(segid 3A4 and resid 246 and name CB)	15.37	0.85	0.84
35	assign (segid 3A4 and resid 190 and name CB)	(segid 3A4 and resid 247 and name CA)	17.01	0.67	0.68
	assign (segid 3A4 and resid 190 and name CB)	(segid 3A4 and resid 247 and name CB)	18.43	0.71	0.70
	assign (segid 3A4 and resid 190 and name CB)	(segid 3A4 and resid 248 and name CA)	15.61	0.64	0.65
	assign (segid 3A4 and resid 190 and name CB)	(segid 3A4 and resid 248 and name CB)	15.61	0.68	0.67
	assign (segid 3A4 and resid 190 and name CB)	(segid 3A4 and resid 249 and name CA)	12.22	0.66	0.66
40	assign (segid 3A4 and resid 190 and name CB)	(segid 3A4 and resid 250 and name CA)	14.17	0.83	0.82
	assign (segid 3A4 and resid 190 and name CB)	(segid 3A4 and resid 250 and name CB)	15.23	0.80	0.81
	assign (segid 3A4 and resid 190 and name CB)	(segid 3A4 and resid 251 and name CA)	16.34	0.87	0.87
	assign (segid 3A4 and resid 190 and name CB)	(segid 3A4 and resid 251 and name CB)	17.23	0.79	0.80
	assign (segid 3A4 and resid 190 and name CB)	(segid 3A4 and resid 252 and name CA)	13.80	1.06	1.07
45	assign (segid 3A4 and resid 190 and name CB)	(segid 3A4 and resid 252 and name CB)	12.79	1.04	1.03
	assign (segid 3A4 and resid 190 and name CB)	(segid 3A4 and resid 253 and name CA)	12.15	1.15	1.14
	assign (segid 3A4 and resid 190 and name CB)	(segid 3A4 and resid 254 and name CA)	15.59	1.13	1.13
	assign (segid 3A4 and resid 190 and name CB)	(segid 3A4 and resid 256 and name CA)	15.68	1.53	1.54
	assign (segid 3A4 and resid 190 and name CB)	(segid 3A4 and resid 257 and name CA)	15.36	1.96	1.96
50	assign (segid 3A4 and resid 190 and name CB)	(segid 3A4 and resid 190 and name C)	2.45	0.03	0.03
	assign (segid 3A4 and resid 190 and name N)	(segid 3A4 and resid 190 and name CA)	1.46	0.01	0.01
	assign (segid 3A4 and resid 190 and name N)	(segid 3A4 and resid 190 and name CB)	2.45	0.04	0.04
	assign (segid 3A4 and resid 190 and name N)	(segid 3A4 and resid 190 and name O)	3.49	0.03	0.03
	assign (segid 3A4 and resid 190 and name N)	(segid 3A4 and resid 191 and name C)	4.67	0.03	0.04
55	assign (segid 3A4 and resid 190 and name N)	(segid 3A4 and resid 191 and name CA)	4.19	0.06	0.07
	assign (segid 3A4 and resid 190 and name N)	(segid 3A4 and resid 191 and name CB)	4.93	0.07	0.07
	assign (segid 3A4 and resid 190 and name N)	(segid 3A4 and resid 191 and name N)	2.80	0.08	0.07
	assign (segid 3A4 and resid 190 and name N)	(segid 3A4 and resid 191 and name O)	5.74	0.04	0.04
	assign (segid 3A4 and resid 190 and name N)	(segid 3A4 and resid 192 and name C)	5.63	0.09	0.08
60	assign (segid 3A4 and resid 190 and name N)	(segid 3A4 and resid 192 and name CA)	5.28	0.12	0.12
	assign (segid 3A4 and resid 190 and name N)	(segid 3A4 and resid 192 and name CB)	5.32	0.25	0.26
	assign (segid 3A4 and resid 190 and name N)	(segid 3A4 and resid 192 and name N)	4.29	0.08	0.08
	assign (segid 3A4 and resid 190 and name N)	(segid 3A4 and resid 192 and name O)	6.84	0.08	0.09
	assign (segid 3A4 and resid 190 and name N)	(segid 3A4 and resid 193 and name C)	6.57	0.09	0.09
65	assign (segid 3A4 and resid 190 and name N)	(segid 3A4 and resid 193 and name CA)	5.65	0.12	0.11
	assign (segid 3A4 and resid 190 and name N)	(segid 3A4 and resid 193 and name CB)	5.09	0.19	0.19
	assign (segid 3A4 and resid 190 and name N)	(segid 3A4 and resid 193 and name N)	4.84	0.09	0.09
	assign (segid 3A4 and resid 190 and name N)	(segid 3A4 and resid 193 and name O)	7.76	0.09	0.10
	assign (segid 3A4 and resid 190 and name N)	(segid 3A4 and resid 194 and name CA)	7.44	0.10	0.10
70	assign (segid 3A4 and resid 190 and name N)	(segid 3A4 and resid 194 and name CB)	7.31	0.14	0.14
	assign (segid 3A4 and resid 190 and name N)	(segid 3A4 and resid 194 and name N)	6.25	0.08	0.09
	assign (segid 3A4 and resid 190 and name O)	(segid 3A4 and resid 190 and name CB)	3.31	0.03	0.03
	assign (segid 3A4 and resid 190 and name O)	(segid 3A4 and resid 191 and name C)	2.91	0.10	0.11
	assign (segid 3A4 and resid 190 and name O)	(segid 3A4 and resid 191 and name CA)	2.78	0.04	0.04
75	assign (segid 3A4 and resid 190 and name O)	(segid 3A4 and resid 191 and name CB)	4.27	0.04	0.05
	assign (segid 3A4 and resid 190 and name O)	(segid 3A4 and resid 191 and name N)	2.26	0.02	0.01
	assign (segid 3A4 and resid 190 and name O)	(segid 3A4 and resid 191 and name O)	3.35	0.12	0.13
	assign (segid 3A4 and resid 190 and name O)	(segid 3A4 and resid 192 and name C)	4.03	0.16	0.16
	assign (segid 3A4 and resid 190 and name O)	(segid 3A4 and resid 192 and name CA)	4.29	0.16	0.15
80	assign (segid 3A4 and resid 190 and name O)	(segid 3A4 and resid 192 and name CB)	5.26	0.20	0.19
	assign (segid 3A4 and resid 190 and name O)	(segid 3A4 and resid 192 and name N)	3.37	0.12	0.13
	assign (segid 3A4 and resid 190 and name O)	(segid 3A4 and resid 192 and name O)	4.98	0.16	0.17

	assign	(segid 3A4 and resid 190 and name O)	(segid 3A4 and resid 193 and name C)	3.84	0.08	0.07
	assign	(segid 3A4 and resid 190 and name O)	(segid 3A4 and resid 193 and name CA)	3.67	0.11	0.10
	assign	(segid 3A4 and resid 190 and name O)	(segid 3A4 and resid 193 and name CB)	3.47	0.15	0.16
	assign	(segid 3A4 and resid 190 and name O)	(segid 3A4 and resid 193 and name N)	3.19	0.14	0.14
5	assign	(segid 3A4 and resid 190 and name O)	(segid 3A4 and resid 193 and name O)	5.04	0.08	0.07
	assign	(segid 3A4 and resid 190 and name O)	(segid 3A4 and resid 194 and name C)	5.14	0.09	0.09
	assign	(segid 3A4 and resid 190 and name O)	(segid 3A4 and resid 194 and name CA)	4.04	0.08	0.09
	assign	(segid 3A4 and resid 190 and name O)	(segid 3A4 and resid 194 and name CB)	3.85	0.13	0.13
	assign	(segid 3A4 and resid 190 and name O)	(segid 3A4 and resid 194 and name N)	3.07	0.07	0.07
10	assign	(segid 3A4 and resid 190 and name O)	(segid 3A4 and resid 194 and name O)	6.28	0.10	0.11
	assign	(segid 3A4 and resid 190 and name O)	(segid 3A4 and resid 195 and name C)	7.25	0.11	0.10
	assign	(segid 3A4 and resid 190 and name O)	(segid 3A4 and resid 195 and name CA)	6.38	0.10	0.11
	assign	(segid 3A4 and resid 190 and name O)	(segid 3A4 and resid 195 and name CB)	6.55	0.13	0.13
	assign	(segid 3A4 and resid 190 and name O)	(segid 3A4 and resid 195 and name N)	5.06	0.09	0.09
15	assign	(segid 3A4 and resid 190 and name O)	(segid 3A4 and resid 196 and name N)	6.89	0.13	0.12
	assign	(segid 3A4 and resid 191 and name C)	(segid 3A4 and resid 191 and name CB)	2.53	0.06	0.05
	assign	(segid 3A4 and resid 191 and name C)	(segid 3A4 and resid 191 and name O)	1.23	0.00	0.01
	assign	(segid 3A4 and resid 191 and name C)	(segid 3A4 and resid 192 and name C)	3.06	0.01	0.02
	assign	(segid 3A4 and resid 191 and name C)	(segid 3A4 and resid 192 and name CA)	2.45	0.02	0.02
20	assign	(segid 3A4 and resid 191 and name C)	(segid 3A4 and resid 192 and name CB)	3.70	0.02	0.01
	assign	(segid 3A4 and resid 191 and name C)	(segid 3A4 and resid 192 and name N)	1.33	0.01	0.01
	assign	(segid 3A4 and resid 191 and name C)	(segid 3A4 and resid 192 and name O)	3.93	0.07	0.07
	assign	(segid 3A4 and resid 191 and name C)	(segid 3A4 and resid 193 and name C)	4.58	0.04	0.04
	assign	(segid 3A4 and resid 191 and name C)	(segid 3A4 and resid 193 and name CA)	4.48	0.07	0.06
25	assign	(segid 3A4 and resid 191 and name C)	(segid 3A4 and resid 193 and name CB)	5.17	0.12	0.12
	assign	(segid 3A4 and resid 191 and name C)	(segid 3A4 and resid 193 and name N)	3.29	0.07	0.07
	assign	(segid 3A4 and resid 191 and name C)	(segid 3A4 and resid 193 and name O)	5.67	0.06	0.05
	assign	(segid 3A4 and resid 191 and name C)	(segid 3A4 and resid 194 and name C)	4.90	0.04	0.05
	assign	(segid 3A4 and resid 191 and name C)	(segid 3A4 and resid 194 and name CA)	4.62	0.02	0.02
30	assign	(segid 3A4 and resid 191 and name C)	(segid 3A4 and resid 194 and name CB)	4.45	0.08	0.09
	assign	(segid 3A4 and resid 191 and name C)	(segid 3A4 and resid 194 and name N)	3.87	0.02	0.03
	assign	(segid 3A4 and resid 191 and name C)	(segid 3A4 and resid 194 and name O)	6.09	0.03	0.04
	assign	(segid 3A4 and resid 191 and name C)	(segid 3A4 and resid 195 and name C)	6.03	0.06	0.05
	assign	(segid 3A4 and resid 191 and name C)	(segid 3A4 and resid 195 and name CA)	4.95	0.05	0.04
35	assign	(segid 3A4 and resid 191 and name C)	(segid 3A4 and resid 195 and name CB)	4.49	0.06	0.07
	assign	(segid 3A4 and resid 191 and name C)	(segid 3A4 and resid 195 and name N)	4.10	0.05	0.05
	assign	(segid 3A4 and resid 191 and name C)	(segid 3A4 and resid 195 and name O)	7.18	0.05	0.05
	assign	(segid 3A4 and resid 191 and name C)	(segid 3A4 and resid 196 and name CA)	7.21	0.11	0.10
	assign	(segid 3A4 and resid 191 and name C)	(segid 3A4 and resid 196 and name CB)	7.27	0.15	0.14
40	assign	(segid 3A4 and resid 191 and name C)	(segid 3A4 and resid 196 and name N)	5.92	0.09	0.08
	assign	(segid 3A4 and resid 191 and name CA)	(segid 3A4 and resid 191 and name C)	1.53	0.01	0.01
	assign	(segid 3A4 and resid 191 and name CA)	(segid 3A4 and resid 191 and name CB)	1.54	0.03	0.03
	assign	(segid 3A4 and resid 191 and name CA)	(segid 3A4 and resid 191 and name O)	2.41	0.01	0.01
	assign	(segid 3A4 and resid 191 and name CA)	(segid 3A4 and resid 192 and name C)	4.46	0.02	0.03
45	assign	(segid 3A4 and resid 191 and name CA)	(segid 3A4 and resid 192 and name CA)	3.82	0.03	0.04
	assign	(segid 3A4 and resid 191 and name CA)	(segid 3A4 and resid 192 and name CB)	4.84	0.01	0.02
	assign	(segid 3A4 and resid 191 and name CA)	(segid 3A4 and resid 192 and name N)	2.44	0.03	0.04
	assign	(segid 3A4 and resid 191 and name CA)	(segid 3A4 and resid 192 and name O)	5.40	0.06	0.06
	assign	(segid 3A4 and resid 191 and name CA)	(segid 3A4 and resid 193 and name C)	5.57	0.06	0.05
50	assign	(segid 3A4 and resid 191 and name CA)	(segid 3A4 and resid 193 and name CA)	5.48	0.09	0.09
	assign	(segid 3A4 and resid 191 and name CA)	(segid 3A4 and resid 193 and name CB)	5.83	0.17	0.17
	assign	(segid 3A4 and resid 191 and name CA)	(segid 3A4 and resid 193 and name N)	4.40	0.09	0.09
	assign	(segid 3A4 and resid 191 and name CA)	(segid 3A4 and resid 193 and name O)	6.71	0.05	0.05
	assign	(segid 3A4 and resid 191 and name CA)	(segid 3A4 and resid 194 and name C)	5.82	0.07	0.07
55	assign	(segid 3A4 and resid 191 and name CA)	(segid 3A4 and resid 194 and name CA)	5.28	0.06	0.05
	assign	(segid 3A4 and resid 191 and name CA)	(segid 3A4 and resid 194 and name CB)	4.71	0.11	0.11
	assign	(segid 3A4 and resid 191 and name CA)	(segid 3A4 and resid 194 and name N)	4.66	0.06	0.06
	assign	(segid 3A4 and resid 191 and name CA)	(segid 3A4 and resid 194 and name O)	7.02	0.06	0.07
	assign	(segid 3A4 and resid 191 and name CA)	(segid 3A4 and resid 195 and name C)	7.34	0.06	0.07
60	assign	(segid 3A4 and resid 191 and name CA)	(segid 3A4 and resid 195 and name CA)	6.15	0.07	0.07
	assign	(segid 3A4 and resid 191 and name CA)	(segid 3A4 and resid 195 and name CB)	5.75	0.08	0.09
	assign	(segid 3A4 and resid 191 and name CA)	(segid 3A4 and resid 195 and name N)	5.20	0.08	0.08
	assign	(segid 3A4 and resid 191 and name CA)	(segid 3A4 and resid 196 and name CA)	8.63	0.09	0.09
	assign	(segid 3A4 and resid 191 and name CA)	(segid 3A4 and resid 196 and name CB)	8.70	0.13	0.13
65	assign	(segid 3A4 and resid 191 and name CA)	(segid 3A4 and resid 196 and name N)	7.32	0.08	0.08
	assign	(segid 3A4 and resid 191 and name CA)	(segid 3A4 and resid 197 and name CA)	10.05	0.10	0.10
	assign	(segid 3A4 and resid 191 and name CA)	(segid 3A4 and resid 197 and name CB)	9.60	0.22	0.23
	assign	(segid 3A4 and resid 191 and name CA)	(segid 3A4 and resid 198 and name CA)	10.74	0.07	0.06
	assign	(segid 3A4 and resid 191 and name CA)	(segid 3A4 and resid 198 and name CB)	9.97	0.09	0.10
70	assign	(segid 3A4 and resid 191 and name CA)	(segid 3A4 and resid 199 and name CA)	12.19	0.20	0.19
	assign	(segid 3A4 and resid 191 and name CA)	(segid 3A4 and resid 199 and name CB)	11.67	0.27	0.27
	assign	(segid 3A4 and resid 191 and name CA)	(segid 3A4 and resid 199 and name N)	14.59	0.28	0.28
	assign	(segid 3A4 and resid 191 and name CA)	(segid 3A4 and resid 200 and name CA)	15.71	0.19	0.20
	assign	(segid 3A4 and resid 191 and name CA)	(segid 3A4 and resid 201 and name CB)	15.06	0.33	0.32
75	assign	(segid 3A4 and resid 191 and name CA)	(segid 3A4 and resid 201 and name CA)	16.43	0.22	0.21
	assign	(segid 3A4 and resid 191 and name CA)	(segid 3A4 and resid 202 and name CB)	15.56	0.32	0.32
	assign	(segid 3A4 and resid 191 and name CA)	(segid 3A4 and resid 202 and name CA)	18.41	0.18	0.17
	assign	(segid 3A4 and resid 191 and name CA)	(segid 3A4 and resid 203 and name CB)	18.02	0.26	0.27
	assign	(segid 3A4 and resid 191 and name CA)	(segid 3A4 and resid 203 and name CA)	18.03	0.79	0.79
80	assign	(segid 3A4 and resid 191 and name CA)	(segid 3A4 and resid 221 and name CB)	16.33	1.51	1.52
	assign	(segid 3A4 and resid 191 and name CA)	(segid 3A4 and resid 241 and name CA)	16.42	1.70	1.70
	assign	(segid 3A4 and resid 191 and name CA)	(segid 3A4 and resid 241 and name CB)	13.67	1.29	1.28
	assign	(segid 3A4 and resid 191 and name CA)	(segid 3A4 and resid 242 and name CA)	13.91	1.26	1.25
	assign	(segid 3A4 and resid 191 and name CA)	(segid 3A4 and resid 242 and name CB)	13.91	1.26	1.25

	assign	(segid 3A4 and resid 191 and name N)	(segid 3A4 and resid 191 and name C)	2.45	0.02	0.03
	assign	(segid 3A4 and resid 191 and name N)	(segid 3A4 and resid 191 and name CA)	1.46	0.01	0.00
	assign	(segid 3A4 and resid 191 and name N)	(segid 3A4 and resid 191 and name CB)	2.46	0.02	0.03
	assign	(segid 3A4 and resid 191 and name N)	(segid 3A4 and resid 191 and name O)	3.48	0.02	0.03
5	assign	(segid 3A4 and resid 191 and name N)	(segid 3A4 and resid 192 and name C)	4.74	0.05	0.04
	assign	(segid 3A4 and resid 191 and name N)	(segid 3A4 and resid 192 and name CA)	4.21	0.05	0.06
	assign	(segid 3A4 and resid 191 and name N)	(segid 3A4 and resid 192 and name CB)	4.94	0.09	0.10
	assign	(segid 3A4 and resid 191 and name N)	(segid 3A4 and resid 192 and name N)	2.82	0.06	0.05
	assign	(segid 3A4 and resid 191 and name N)	(segid 3A4 and resid 192 and name O)	5.84	0.05	0.06
10	assign	(segid 3A4 and resid 191 and name N)	(segid 3A4 and resid 193 and name C)	5.70	0.06	0.06
	assign	(segid 3A4 and resid 191 and name N)	(segid 3A4 and resid 193 and name CA)	5.33	0.10	0.11
	assign	(segid 3A4 and resid 191 and name N)	(segid 3A4 and resid 193 and name CB)	5.33	0.20	0.19
	assign	(segid 3A4 and resid 191 and name N)	(segid 3A4 and resid 193 and name N)	4.33	0.09	0.08
	assign	(segid 3A4 and resid 191 and name N)	(segid 3A4 and resid 193 and name O)	6.92	0.06	0.06
15	assign	(segid 3A4 and resid 191 and name N)	(segid 3A4 and resid 194 and name C)	6.58	0.04	0.04
	assign	(segid 3A4 and resid 191 and name N)	(segid 3A4 and resid 194 and name CA)	5.78	0.04	0.04
	assign	(segid 3A4 and resid 191 and name N)	(segid 3A4 and resid 194 and name CB)	5.31	0.11	0.10
	assign	(segid 3A4 and resid 191 and name N)	(segid 3A4 and resid 194 and name N)	4.93	0.04	0.04
	assign	(segid 3A4 and resid 191 and name N)	(segid 3A4 and resid 194 and name O)	7.79	0.03	0.04
20	assign	(segid 3A4 and resid 191 and name N)	(segid 3A4 and resid 195 and name C)	7.20	0.05	0.05
	assign	(segid 3A4 and resid 191 and name N)	(segid 3A4 and resid 195 and name CB)	6.91	0.08	0.08
	assign	(segid 3A4 and resid 191 and name N)	(segid 3A4 and resid 195 and name N)	6.12	0.05	0.05
	assign	(segid 3A4 and resid 191 and name O)	(segid 3A4 and resid 191 and name CB)	3.35	0.06	0.05
	assign	(segid 3A4 and resid 191 and name O)	(segid 3A4 and resid 192 and name C)	3.01	0.05	0.05
25	assign	(segid 3A4 and resid 191 and name O)	(segid 3A4 and resid 192 and name CA)	2.78	0.02	0.02
	assign	(segid 3A4 and resid 191 and name O)	(segid 3A4 and resid 192 and name CB)	4.25	0.03	0.02
	assign	(segid 3A4 and resid 191 and name O)	(segid 3A4 and resid 192 and name N)	2.24	0.01	0.01
	assign	(segid 3A4 and resid 191 and name O)	(segid 3A4 and resid 192 and name O)	3.52	0.12	0.13
	assign	(segid 3A4 and resid 191 and name O)	(segid 3A4 and resid 193 and name C)	4.10	0.05	0.05
30	assign	(segid 3A4 and resid 191 and name O)	(segid 3A4 and resid 193 and name CA)	4.36	0.05	0.06
	assign	(segid 3A4 and resid 191 and name O)	(segid 3A4 and resid 193 and name CB)	5.28	0.10	0.09
	assign	(segid 3A4 and resid 191 and name O)	(segid 3A4 and resid 193 and name N)	3.41	0.05	0.04
	assign	(segid 3A4 and resid 191 and name O)	(segid 3A4 and resid 193 and name O)	5.03	0.08	0.09
	assign	(segid 3A4 and resid 191 and name O)	(segid 3A4 and resid 194 and name C)	3.81	0.06	0.06
35	assign	(segid 3A4 and resid 191 and name O)	(segid 3A4 and resid 194 and name CA)	3.76	0.04	0.04
	assign	(segid 3A4 and resid 191 and name O)	(segid 3A4 and resid 194 and name CB)	3.67	0.09	0.09
	assign	(segid 3A4 and resid 191 and name O)	(segid 3A4 and resid 194 and name N)	3.30	0.04	0.03
	assign	(segid 3A4 and resid 191 and name O)	(segid 3A4 and resid 194 and name O)	4.98	0.05	0.05
	assign	(segid 3A4 and resid 191 and name O)	(segid 3A4 and resid 195 and name C)	4.95	0.08	0.08
40	assign	(segid 3A4 and resid 191 and name O)	(segid 3A4 and resid 195 and name CA)	3.78	0.06	0.06
	assign	(segid 3A4 and resid 191 and name O)	(segid 3A4 and resid 195 and name CB)	3.47	0.07	0.07
	assign	(segid 3A4 and resid 191 and name O)	(segid 3A4 and resid 195 and name N)	2.94	0.08	0.07
	assign	(segid 3A4 and resid 191 and name O)	(segid 3A4 and resid 195 and name O)	6.07	0.07	0.07
	assign	(segid 3A4 and resid 191 and name O)	(segid 3A4 and resid 196 and name C)	7.22	0.10	0.11
45	assign	(segid 3A4 and resid 191 and name O)	(segid 3A4 and resid 196 and name CA)	6.37	0.12	0.12
	assign	(segid 3A4 and resid 191 and name O)	(segid 3A4 and resid 196 and name CB)	6.64	0.15	0.15
	assign	(segid 3A4 and resid 191 and name O)	(segid 3A4 and resid 196 and name N)	5.00	0.11	0.10
	assign	(segid 3A4 and resid 191 and name O)	(segid 3A4 and resid 197 and name N)	6.93	0.09	0.08
	assign	(segid 3A4 and resid 191 and name O)	(segid 3A4 and resid 198 and name CG)	7.66	0.16	0.16
50	assign	(segid 3A4 and resid 191 and name O)	(segid 3A4 and resid 198 and name N)	7.78	0.06	0.07
	assign	(segid 3A4 and resid 192 and name C)	(segid 3A4 and resid 192 and name CB)	2.51	0.04	0.04
	assign	(segid 3A4 and resid 192 and name C)	(segid 3A4 and resid 192 and name O)	1.24	0.01	0.00
	assign	(segid 3A4 and resid 192 and name C)	(segid 3A4 and resid 193 and name C)	3.04	0.05	0.04
	assign	(segid 3A4 and resid 192 and name C)	(segid 3A4 and resid 193 and name CA)	2.45	0.04	0.04
55	assign	(segid 3A4 and resid 192 and name C)	(segid 3A4 and resid 193 and name CB)	3.72	0.05	0.05
	assign	(segid 3A4 and resid 192 and name C)	(segid 3A4 and resid 193 and name N)	1.33	0.01	0.01
	assign	(segid 3A4 and resid 192 and name C)	(segid 3A4 and resid 193 and name O)	3.85	0.09	0.09
	assign	(segid 3A4 and resid 192 and name C)	(segid 3A4 and resid 194 and name C)	4.50	0.05	0.04
	assign	(segid 3A4 and resid 192 and name C)	(segid 3A4 and resid 194 and name CA)	4.50	0.03	0.03
	assign	(segid 3A4 and resid 192 and name C)	(segid 3A4 and resid 194 and name CB)	5.30	0.07	0.08
60	assign	(segid 3A4 and resid 192 and name C)	(segid 3A4 and resid 194 and name N)	3.34	0.03	0.03
	assign	(segid 3A4 and resid 192 and name C)	(segid 3A4 and resid 194 and name O)	5.47	0.11	0.11
	assign	(segid 3A4 and resid 192 and name C)	(segid 3A4 and resid 195 and name C)	4.73	0.07	0.08
	assign	(segid 3A4 and resid 192 and name C)	(segid 3A4 and resid 195 and name CA)	4.43	0.07	0.08
65	assign	(segid 3A4 and resid 192 and name C)	(segid 3A4 and resid 195 and name CB)	4.25	0.06	0.07
	assign	(segid 3A4 and resid 192 and name C)	(segid 3A4 and resid 195 and name N)	3.78	0.07	0.07
	assign	(segid 3A4 and resid 192 and name C)	(segid 3A4 and resid 195 and name O)	5.93	0.06	0.07
	assign	(segid 3A4 and resid 192 and name C)	(segid 3A4 and resid 196 and name C)	6.02	0.12	0.12
	assign	(segid 3A4 and resid 192 and name C)	(segid 3A4 and resid 196 and name CA)	4.91	0.12	0.12
70	assign	(segid 3A4 and resid 192 and name C)	(segid 3A4 and resid 196 and name CB)	4.54	0.17	0.17
	assign	(segid 3A4 and resid 192 and name C)	(segid 3A4 and resid 196 and name N)	4.00	0.08	0.09
	assign	(segid 3A4 and resid 192 and name C)	(segid 3A4 and resid 196 and name O)	7.17	0.12	0.12
	assign	(segid 3A4 and resid 192 and name C)	(segid 3A4 and resid 197 and name CA)	7.20	0.08	0.08
	assign	(segid 3A4 and resid 192 and name C)	(segid 3A4 and resid 197 and name CB)	7.22	0.07	0.07
	assign	(segid 3A4 and resid 192 and name C)	(segid 3A4 and resid 197 and name N)	5.91	0.10	0.11
75	assign	(segid 3A4 and resid 192 and name C)	(segid 3A4 and resid 198 and name N)	7.78	0.09	0.09
	assign	(segid 3A4 and resid 192 and name C)	(segid 3A4 and resid 192 and name C)	1.52	0.01	0.01
	assign	(segid 3A4 and resid 192 and name CA)	(segid 3A4 and resid 192 and name CB)	1.52	0.01	0.02
	assign	(segid 3A4 and resid 192 and name CA)	(segid 3A4 and resid 192 and name O)	2.40	0.01	0.00
80	assign	(segid 3A4 and resid 192 and name CA)	(segid 3A4 and resid 193 and name C)	4.41	0.04	0.05
	assign	(segid 3A4 and resid 192 and name CA)	(segid 3A4 and resid 193 and name CA)	3.82	0.04	0.03
	assign	(segid 3A4 and resid 192 and name CA)	(segid 3A4 and resid 193 and name CB)	4.86	0.07	0.06
	assign	(segid 3A4 and resid 192 and name CA)	(segid 3A4 and resid 193 and name N)	2.43	0.03	0.03

	assign (segid 3A4 and resid 192 and name CA) (segid 3A4 and resid 193 and name O)	5.30	0.08	0.09
	assign (segid 3A4 and resid 192 and name CA) (segid 3A4 and resid 194 and name C)	5.42	0.05	0.05
	assign (segid 3A4 and resid 192 and name CA) (segid 3A4 and resid 194 and name CA)	5.47	0.03	0.03
	assign (segid 3A4 and resid 192 and name CA) (segid 3A4 and resid 194 and name CB)	5.95	0.08	0.08
5	assign (segid 3A4 and resid 192 and name CA) (segid 3A4 and resid 194 and name N)	4.41	0.03	0.04
	assign (segid 3A4 and resid 192 and name CA) (segid 3A4 and resid 194 and name O)	6.47	0.09	0.09
	assign (segid 3A4 and resid 192 and name CA) (segid 3A4 and resid 195 and name C)	5.51	0.09	0.08
	assign (segid 3A4 and resid 192 and name CA) (segid 3A4 and resid 195 and name CA)	4.96	0.08	0.08
	assign (segid 3A4 and resid 192 and name CA) (segid 3A4 and resid 195 and name CB)	4.32	0.10	0.11
10	assign (segid 3A4 and resid 192 and name CA) (segid 3A4 and resid 195 and name N)	4.47	0.07	0.07
	assign (segid 3A4 and resid 192 and name CA) (segid 3A4 and resid 195 and name O)	6.68	0.09	0.08
	assign (segid 3A4 and resid 192 and name CA) (segid 3A4 and resid 196 and name C)	7.24	0.14	0.14
	assign (segid 3A4 and resid 192 and name CA) (segid 3A4 and resid 196 and name CA)	6.02	0.15	0.15
	assign (segid 3A4 and resid 192 and name CA) (segid 3A4 and resid 196 and name CB)	5.75	0.20	0.21
15	assign (segid 3A4 and resid 192 and name CA) (segid 3A4 and resid 196 and name N)	5.01	0.12	0.13
	assign (segid 3A4 and resid 192 and name CA) (segid 3A4 and resid 197 and name CA)	8.55	0.09	0.09
	assign (segid 3A4 and resid 192 and name CA) (segid 3A4 and resid 197 and name CB)	8.60	0.10	0.10
	assign (segid 3A4 and resid 192 and name CA) (segid 3A4 and resid 197 and name N)	7.24	0.11	0.11
	assign (segid 3A4 and resid 192 and name CA) (segid 3A4 and resid 198 and name CA)	9.86	0.13	0.12
20	assign (segid 3A4 and resid 192 and name CA) (segid 3A4 and resid 198 and name CB)	9.49	0.17	0.17
	assign (segid 3A4 and resid 192 and name CA) (segid 3A4 and resid 199 and name CA)	10.31	0.11	0.12
	assign (segid 3A4 and resid 192 and name CA) (segid 3A4 and resid 199 and name CB)	9.46	0.18	0.17
	assign (segid 3A4 and resid 192 and name CA) (segid 3A4 and resid 200 and name CA)	12.45	0.35	0.36
	assign (segid 3A4 and resid 192 and name CA) (segid 3A4 and resid 201 and name CA)	14.38	0.25	0.26
25	assign (segid 3A4 and resid 192 and name CA) (segid 3A4 and resid 201 and name CB)	14.06	0.35	0.36
	assign (segid 3A4 and resid 192 and name CA) (segid 3A4 and resid 202 and name CA)	15.13	0.13	0.14
	assign (segid 3A4 and resid 192 and name CA) (segid 3A4 and resid 202 and name CB)	14.29	0.22	0.23
	assign (segid 3A4 and resid 192 and name CA) (segid 3A4 and resid 203 and name CA)	16.41	0.13	0.14
	assign (segid 3A4 and resid 192 and name CA) (segid 3A4 and resid 203 and name CB)	15.78	0.28	0.27
30	assign (segid 3A4 and resid 192 and name CA) (segid 3A4 and resid 203 and name N)	18.48	0.22	0.22
	assign (segid 3A4 and resid 192 and name CA) (segid 3A4 and resid 204 and name CA)	18.12	0.21	0.21
	assign (segid 3A4 and resid 192 and name CA) (segid 3A4 and resid 204 and name CB)	19.15	0.16	0.16
	assign (segid 3A4 and resid 192 and name CA) (segid 3A4 and resid 205 and name CA)	17.94	0.75	0.75
	assign (segid 3A4 and resid 192 and name CA) (segid 3A4 and resid 221 and name CB)	15.17	1.45	1.45
35	assign (segid 3A4 and resid 192 and name CA) (segid 3A4 and resid 241 and name CB)	14.92	1.67	1.67
	assign (segid 3A4 and resid 192 and name CA) (segid 3A4 and resid 241 and name N)	12.90	1.07	1.07
	assign (segid 3A4 and resid 192 and name CA) (segid 3A4 and resid 242 and name CA)	13.08	1.03	1.03
	assign (segid 3A4 and resid 192 and name CA) (segid 3A4 and resid 242 and name CB)	15.08	0.80	0.80
	assign (segid 3A4 and resid 192 and name CA) (segid 3A4 and resid 243 and name CA)	16.57	0.82	0.81
40	assign (segid 3A4 and resid 192 and name CA) (segid 3A4 and resid 243 and name CB)	15.18	0.87	0.88
	assign (segid 3A4 and resid 192 and name CA) (segid 3A4 and resid 244 and name CA)	15.64	1.01	1.02
	assign (segid 3A4 and resid 192 and name CA) (segid 3A4 and resid 244 and name CB)	11.52	0.81	0.81
	assign (segid 3A4 and resid 192 and name CA) (segid 3A4 and resid 245 and name CA)	10.49	0.94	0.93
	assign (segid 3A4 and resid 192 and name CA) (segid 3A4 and resid 245 and name CB)	11.80	0.55	0.55
45	assign (segid 3A4 and resid 192 and name CA) (segid 3A4 and resid 246 and name CA)	12.33	0.56	0.55
	assign (segid 3A4 and resid 192 and name CA) (segid 3A4 and resid 246 and name CB)	14.91	0.55	0.56
	assign (segid 3A4 and resid 192 and name CA) (segid 3A4 and resid 247 and name CA)	16.11	0.58	0.57
	assign (segid 3A4 and resid 192 and name CA) (segid 3A4 and resid 247 and name CB)	13.81	0.52	0.51
	assign (segid 3A4 and resid 192 and name CA) (segid 3A4 and resid 248 and name CA)	13.38	0.53	0.52
50	assign (segid 3A4 and resid 192 and name CA) (segid 3A4 and resid 248 and name CB)	11.21	0.69	0.70
	assign (segid 3A4 and resid 192 and name CA) (segid 3A4 and resid 249 and name CA)	14.07	0.80	0.79
	assign (segid 3A4 and resid 192 and name CA) (segid 3A4 and resid 250 and name CA)	14.83	0.71	0.71
	assign (segid 3A4 and resid 192 and name CA) (segid 3A4 and resid 250 and name CB)	16.51	0.80	0.79
	assign (segid 3A4 and resid 192 and name CA) (segid 3A4 and resid 251 and name CA)	16.99	0.72	0.71
55	assign (segid 3A4 and resid 192 and name CA) (segid 3A4 and resid 251 and name CB)	14.79	1.02	1.01
	assign (segid 3A4 and resid 192 and name CA) (segid 3A4 and resid 252 and name CA)	13.51	1.03	1.02
	assign (segid 3A4 and resid 192 and name CA) (segid 3A4 and resid 252 and name CB)	14.32	1.15	1.15
	assign (segid 3A4 and resid 192 and name CA) (segid 3A4 and resid 253 and name CA)	17.64	1.10	1.10
	assign (segid 3A4 and resid 192 and name CA) (segid 3A4 and resid 254 and name CA)	5.46	0.07	0.08
60	assign (segid 3A4 and resid 192 and name CB) (segid 3A4 and resid 193 and name C)	4.53	0.09	0.10
	assign (segid 3A4 and resid 192 and name CB) (segid 3A4 and resid 193 and name CB)	5.41	0.14	0.13
	assign (segid 3A4 and resid 192 and name CB) (segid 3A4 and resid 193 and name N)	3.20	0.09	0.09
	assign (segid 3A4 and resid 192 and name CB) (segid 3A4 and resid 193 and name O)	6.30	0.10	0.11
	assign (segid 3A4 and resid 192 and name CB) (segid 3A4 and resid 194 and name C)	6.83	0.06	0.07
65	assign (segid 3A4 and resid 192 and name CB) (segid 3A4 and resid 194 and name CA)	6.84	0.03	0.04
	assign (segid 3A4 and resid 192 and name CB) (segid 3A4 and resid 194 and name CB)	7.39	0.09	0.08
	assign (segid 3A4 and resid 192 and name CB) (segid 3A4 and resid 194 and name N)	5.68	0.05	0.05
	assign (segid 3A4 and resid 192 and name CB) (segid 3A4 and resid 195 and name CA)	6.64	0.14	0.14
	assign (segid 3A4 and resid 192 and name CB) (segid 3A4 and resid 195 and name CB)	6.28	0.13	0.13
70	assign (segid 3A4 and resid 192 and name CB) (segid 3A4 and resid 195 and name N)	5.54	0.17	0.17
	assign (segid 3A4 and resid 192 and name CB) (segid 3A4 and resid 195 and name O)	5.91	0.10	0.09
	assign (segid 3A4 and resid 192 and name CB) (segid 3A4 and resid 196 and name CA)	6.78	0.18	0.17
	assign (segid 3A4 and resid 192 and name CB) (segid 3A4 and resid 196 and name CB)	6.25	0.20	0.21
	assign (segid 3A4 and resid 192 and name CB) (segid 3A4 and resid 196 and name N)	6.00	0.15	0.14
75	assign (segid 3A4 and resid 192 and name CB) (segid 3A4 and resid 197 and name CA)	9.56	0.10	0.11
	assign (segid 3A4 and resid 192 and name CB) (segid 3A4 and resid 197 and name CB)	9.69	0.09	0.08
	assign (segid 3A4 and resid 192 and name CB) (segid 3A4 and resid 198 and name CA)	11.10	0.16	0.15
	assign (segid 3A4 and resid 192 and name CB) (segid 3A4 and resid 198 and name CB)	10.82	0.21	0.21
	assign (segid 3A4 and resid 192 and name CB) (segid 3A4 and resid 199 and name CA)	11.25	0.15	0.14
80	assign (segid 3A4 and resid 192 and name CB) (segid 3A4 and resid 199 and name CB)	10.26	0.17	0.17
	assign (segid 3A4 and resid 192 and name CB) (segid 3A4 and resid 200 and name CA)	13.24	0.37	0.37
	assign (segid 3A4 and resid 192 and name CB) (segid 3A4 and resid 201 and name CA)	15.44	0.29	0.28
	assign (segid 3A4 and resid 192 and name CB) (segid 3A4 and resid 201 and name CB)	15.22	0.37	0.36

	assign (segid 3A4 and resid 192 and name CB)	(segid 3A4 and resid 202 and name CA)	16.19	0.18	0.18
	assign (segid 3A4 and resid 192 and name CB)	(segid 3A4 and resid 202 and name CB)	15.35	0.26	0.26
	assign (segid 3A4 and resid 192 and name CB)	(segid 3A4 and resid 203 and name CA)	17.21	0.13	0.13
	assign (segid 3A4 and resid 192 and name CB)	(segid 3A4 and resid 203 and name CB)	16.47	0.26	0.26
5	assign (segid 3A4 and resid 192 and name CB)	(segid 3A4 and resid 204 and name CA)	19.33	0.24	0.25
	assign (segid 3A4 and resid 192 and name CB)	(segid 3A4 and resid 204 and name CB)	18.99	0.23	0.23
	assign (segid 3A4 and resid 192 and name CB)	(segid 3A4 and resid 241 and name CA)	16.03	1.45	1.45
	assign (segid 3A4 and resid 192 and name CB)	(segid 3A4 and resid 241 and name CB)	15.69	1.67	1.67
	assign (segid 3A4 and resid 192 and name CB)	(segid 3A4 and resid 242 and name CA)	13.74	1.08	1.09
	assign (segid 3A4 and resid 192 and name CB)	(segid 3A4 and resid 242 and name CB)	13.80	1.06	1.06
10	assign (segid 3A4 and resid 192 and name CB)	(segid 3A4 and resid 243 and name CA)	16.11	0.84	0.83
	assign (segid 3A4 and resid 192 and name CB)	(segid 3A4 and resid 243 and name CB)	17.58	0.85	0.86
	assign (segid 3A4 and resid 192 and name CB)	(segid 3A4 and resid 244 and name CA)	16.38	0.89	0.89
	assign (segid 3A4 and resid 192 and name CB)	(segid 3A4 and resid 244 and name CB)	16.80	1.02	1.02
	assign (segid 3A4 and resid 192 and name CB)	(segid 3A4 and resid 245 and name CA)	12.76	0.80	0.81
15	assign (segid 3A4 and resid 192 and name CB)	(segid 3A4 and resid 245 and name CB)	11.65	0.91	0.91
	assign (segid 3A4 and resid 192 and name CB)	(segid 3A4 and resid 246 and name CA)	13.04	0.61	0.61
	assign (segid 3A4 and resid 192 and name CB)	(segid 3A4 and resid 246 and name CB)	13.48	0.63	0.62
	assign (segid 3A4 and resid 192 and name CB)	(segid 3A4 and resid 247 and name CA)	16.27	0.61	0.60
	assign (segid 3A4 and resid 192 and name CB)	(segid 3A4 and resid 247 and name CB)	17.45	0.62	0.61
20	assign (segid 3A4 and resid 192 and name CB)	(segid 3A4 and resid 248 and name CA)	15.25	0.53	0.53
	assign (segid 3A4 and resid 192 and name CB)	(segid 3A4 and resid 248 and name CB)	14.80	0.52	0.52
	assign (segid 3A4 and resid 192 and name CB)	(segid 3A4 and resid 249 and name CA)	12.67	0.71	0.72
	assign (segid 3A4 and resid 192 and name CB)	(segid 3A4 and resid 250 and name CA)	15.48	0.83	0.82
	assign (segid 3A4 and resid 192 and name CB)	(segid 3A4 and resid 250 and name CB)	16.21	0.76	0.75
25	assign (segid 3A4 and resid 192 and name CB)	(segid 3A4 and resid 251 and name CA)	17.98	0.80	0.81
	assign (segid 3A4 and resid 192 and name CB)	(segid 3A4 and resid 251 and name CB)	18.47	0.72	0.72
	assign (segid 3A4 and resid 192 and name CB)	(segid 3A4 and resid 252 and name CA)	16.26	0.99	0.99
	assign (segid 3A4 and resid 192 and name CB)	(segid 3A4 and resid 252 and name CB)	14.98	1.00	1.00
	assign (segid 3A4 and resid 192 and name CB)	(segid 3A4 and resid 253 and name CA)	15.70	1.13	1.14
30	assign (segid 3A4 and resid 192 and name N)	(segid 3A4 and resid 192 and name C)	2.48	0.01	0.01
	assign (segid 3A4 and resid 192 and name N)	(segid 3A4 and resid 192 and name CA)	1.46	0.00	0.00
	assign (segid 3A4 and resid 192 and name N)	(segid 3A4 and resid 192 and name CB)	2.43	0.02	0.03
	assign (segid 3A4 and resid 192 and name N)	(segid 3A4 and resid 192 and name O)	3.52	0.02	0.03
	assign (segid 3A4 and resid 192 and name N)	(segid 3A4 and resid 193 and name C)	4.73	0.03	0.03
35	assign (segid 3A4 and resid 192 and name N)	(segid 3A4 and resid 193 and name CA)	4.22	0.05	0.05
	assign (segid 3A4 and resid 192 and name N)	(segid 3A4 and resid 193 and name CB)	4.95	0.10	0.10
	assign (segid 3A4 and resid 192 and name N)	(segid 3A4 and resid 193 and name N)	2.81	0.05	0.06
	assign (segid 3A4 and resid 192 and name N)	(segid 3A4 and resid 193 and name O)	5.81	0.06	0.05
	assign (segid 3A4 and resid 192 and name N)	(segid 3A4 and resid 194 and name C)	5.61	0.04	0.03
40	assign (segid 3A4 and resid 192 and name N)	(segid 3A4 and resid 194 and name CA)	5.38	0.03	0.02
	assign (segid 3A4 and resid 192 and name N)	(segid 3A4 and resid 194 and name CB)	5.50	0.10	0.10
	assign (segid 3A4 and resid 192 and name N)	(segid 3A4 and resid 194 and name N)	4.37	0.03	0.03
	assign (segid 3A4 and resid 192 and name N)	(segid 3A4 and resid 194 and name O)	6.77	0.04	0.04
	assign (segid 3A4 and resid 192 and name N)	(segid 3A4 and resid 195 and name C)	6.30	0.05	0.06
45	assign (segid 3A4 and resid 192 and name N)	(segid 3A4 and resid 195 and name CA)	5.47	0.04	0.03
	assign (segid 3A4 and resid 192 and name N)	(segid 3A4 and resid 195 and name CB)	4.87	0.06	0.07
	assign (segid 3A4 and resid 192 and name N)	(segid 3A4 and resid 195 and name N)	4.75	0.04	0.04
	assign (segid 3A4 and resid 192 and name N)	(segid 3A4 and resid 195 and name O)	7.49	0.05	0.05
	assign (segid 3A4 and resid 192 and name N)	(segid 3A4 and resid 196 and name CA)	7.12	0.13	0.13
50	assign (segid 3A4 and resid 192 and name N)	(segid 3A4 and resid 196 and name CB)	6.95	0.18	0.18
	assign (segid 3A4 and resid 192 and name N)	(segid 3A4 and resid 196 and name N)	5.97	0.10	0.11
	assign (segid 3A4 and resid 192 and name O)	(segid 3A4 and resid 192 and name CB)	3.29	0.07	0.07
	assign (segid 3A4 and resid 192 and name O)	(segid 3A4 and resid 193 and name C)	3.00	0.07	0.07
	assign (segid 3A4 and resid 192 and name O)	(segid 3A4 and resid 193 and name CA)	2.79	0.05	0.05
55	assign (segid 3A4 and resid 192 and name O)	(segid 3A4 and resid 193 and name CB)	4.27	0.05	0.06
	assign (segid 3A4 and resid 192 and name O)	(segid 3A4 and resid 193 and name N)	2.25	0.01	0.00
	assign (segid 3A4 and resid 192 and name O)	(segid 3A4 and resid 193 and name O)	3.44	0.12	0.13
	assign (segid 3A4 and resid 192 and name O)	(segid 3A4 and resid 194 and name C)	4.08	0.10	0.09
60	assign (segid 3A4 and resid 192 and name O)	(segid 3A4 and resid 194 and name CA)	4.44	0.08	0.08
	assign (segid 3A4 and resid 192 and name O)	(segid 3A4 and resid 194 and name CB)	5.46	0.12	0.12
	assign (segid 3A4 and resid 192 and name O)	(segid 3A4 and resid 194 and name N)	3.51	0.06	0.07
	assign (segid 3A4 and resid 192 and name O)	(segid 3A4 and resid 194 and name O)	4.87	0.16	0.16
	assign (segid 3A4 and resid 192 and name O)	(segid 3A4 and resid 195 and name C)	3.71	0.09	0.09
	assign (segid 3A4 and resid 192 and name O)	(segid 3A4 and resid 195 and name CA)	3.71	0.12	0.13
65	assign (segid 3A4 and resid 192 and name O)	(segid 3A4 and resid 195 and name CB)	3.67	0.11	0.10
	assign (segid 3A4 and resid 192 and name O)	(segid 3A4 and resid 195 and name N)	3.33	0.12	0.13
	assign (segid 3A4 and resid 192 and name O)	(segid 3A4 and resid 195 and name O)	4.88	0.08	0.07
	assign (segid 3A4 and resid 192 and name O)	(segid 3A4 and resid 196 and name C)	4.90	0.12	0.12
	assign (segid 3A4 and resid 192 and name O)	(segid 3A4 and resid 196 and name CA)	3.72	0.12	0.12
70	assign (segid 3A4 and resid 192 and name O)	(segid 3A4 and resid 196 and name CB)	3.45	0.21	0.20
	assign (segid 3A4 and resid 192 and name O)	(segid 3A4 and resid 196 and name N)	2.87	0.07	0.06
	assign (segid 3A4 and resid 192 and name O)	(segid 3A4 and resid 196 and name O)	6.02	0.13	0.12
	assign (segid 3A4 and resid 192 and name O)	(segid 3A4 and resid 197 and name C)	7.15	0.07	0.08
	assign (segid 3A4 and resid 192 and name O)	(segid 3A4 and resid 197 and name CA)	6.31	0.08	0.08
75	assign (segid 3A4 and resid 192 and name O)	(segid 3A4 and resid 197 and name CB)	6.54	0.05	0.05
	assign (segid 3A4 and resid 192 and name O)	(segid 3A4 and resid 197 and name N)	4.95	0.10	0.09
	assign (segid 3A4 and resid 192 and name O)	(segid 3A4 and resid 198 and name C)	6.87	0.06	0.05
	assign (segid 3A4 and resid 192 and name O)	(segid 3A4 and resid 199 and name CB)	7.58	0.16	0.15
	assign (segid 3A4 and resid 192 and name O)	(segid 3A4 and resid 199 and name N)	7.66	0.05	0.06
80	assign (segid 3A4 and resid 193 and name C)	(segid 3A4 and resid 193 and name CB)	2.50	0.02	0.02
	assign (segid 3A4 and resid 193 and name C)	(segid 3A4 and resid 193 and name O)	1.24	0.01	0.00
	assign (segid 3A4 and resid 193 and name C)	(segid 3A4 and resid 194 and name C)	3.00	0.06	0.05

	assign (segid 3A4 and resid 193 and name C) (segid 3A4 and resid 194 and name CA)	2.44	0.02	0.01
	assign (segid 3A4 and resid 193 and name C) (segid 3A4 and resid 194 and name CB)	3.74	0.02	0.02
	assign (segid 3A4 and resid 193 and name C) (segid 3A4 and resid 194 and name N)	1.34	0.01	0.00
	assign (segid 3A4 and resid 193 and name C) (segid 3A4 and resid 194 and name O)	3.76	0.15	0.15
	assign (segid 3A4 and resid 193 and name C) (segid 3A4 and resid 195 and name C)	4.58	0.06	0.06
5	assign (segid 3A4 and resid 193 and name C) (segid 3A4 and resid 195 and name CA)	4.48	0.07	0.06
	assign (segid 3A4 and resid 193 and name C) (segid 3A4 and resid 195 and name CB)	5.25	0.06	0.06
	assign (segid 3A4 and resid 193 and name C) (segid 3A4 and resid 195 and name N)	3.31	0.08	0.08
	assign (segid 3A4 and resid 193 and name C) (segid 3A4 and resid 195 and name O)	5.66	0.06	0.05
	assign (segid 3A4 and resid 193 and name C) (segid 3A4 and resid 196 and name C)	4.93	0.05	0.06
10	assign (segid 3A4 and resid 193 and name C) (segid 3A4 and resid 196 and name CA)	4.58	0.08	0.09
	assign (segid 3A4 and resid 193 and name C) (segid 3A4 and resid 196 and name CB)	4.37	0.10	0.10
	assign (segid 3A4 and resid 193 and name C) (segid 3A4 and resid 196 and name N)	3.84	0.08	0.09
	assign (segid 3A4 and resid 193 and name C) (segid 3A4 and resid 196 and name O)	6.14	0.05	0.06
	assign (segid 3A4 and resid 193 and name C) (segid 3A4 and resid 197 and name C)	6.19	0.09	0.08
15	assign (segid 3A4 and resid 193 and name C) (segid 3A4 and resid 197 and name CA)	5.10	0.06	0.07
	assign (segid 3A4 and resid 193 and name C) (segid 3A4 and resid 197 and name CB)	4.66	0.10	0.09
	assign (segid 3A4 and resid 193 and name C) (segid 3A4 and resid 197 and name CG)	5.99	0.12	0.12
	assign (segid 3A4 and resid 193 and name C) (segid 3A4 and resid 197 and name N)	4.21	0.07	0.06
	assign (segid 3A4 and resid 193 and name C) (segid 3A4 and resid 197 and name O)	7.36	0.09	0.08
20	assign (segid 3A4 and resid 193 and name C) (segid 3A4 and resid 198 and name CA)	7.34	0.12	0.13
	assign (segid 3A4 and resid 193 and name C) (segid 3A4 and resid 198 and name CB)	7.36	0.13	0.12
	assign (segid 3A4 and resid 193 and name C) (segid 3A4 and resid 198 and name CG)	7.12	0.25	0.25
	assign (segid 3A4 and resid 193 and name C) (segid 3A4 and resid 198 and name N)	6.06	0.12	0.12
	assign (segid 3A4 and resid 193 and name C) (segid 3A4 and resid 198 and name O)	1.52	0.01	0.01
25	assign (segid 3A4 and resid 193 and name CA) (segid 3A4 and resid 193 and name CB)	1.53	0.01	0.02
	assign (segid 3A4 and resid 193 and name CA) (segid 3A4 and resid 193 and name O)	2.39	0.01	0.01
	assign (segid 3A4 and resid 193 and name CA) (segid 3A4 and resid 194 and name C)	4.38	0.05	0.04
	assign (segid 3A4 and resid 193 and name CA) (segid 3A4 and resid 194 and name CB)	3.81	0.01	0.02
	assign (segid 3A4 and resid 193 and name CA) (segid 3A4 and resid 194 and name N)	4.90	0.03	0.03
30	assign (segid 3A4 and resid 193 and name CA) (segid 3A4 and resid 194 and name O)	2.44	0.01	0.02
	assign (segid 3A4 and resid 193 and name CA) (segid 3A4 and resid 195 and name C)	5.20	0.15	0.15
	assign (segid 3A4 and resid 193 and name CA) (segid 3A4 and resid 195 and name CB)	5.50	0.09	0.08
	assign (segid 3A4 and resid 193 and name CA) (segid 3A4 and resid 195 and name N)	5.43	0.09	0.09
35	assign (segid 3A4 and resid 193 and name CA) (segid 3A4 and resid 195 and name O)	5.88	0.07	0.06
	assign (segid 3A4 and resid 193 and name CA) (segid 3A4 and resid 196 and name C)	4.38	0.09	0.09
	assign (segid 3A4 and resid 193 and name CA) (segid 3A4 and resid 196 and name CB)	6.63	0.07	0.07
	assign (segid 3A4 and resid 193 and name CA) (segid 3A4 and resid 196 and name N)	5.77	0.05	0.05
	assign (segid 3A4 and resid 193 and name CA) (segid 3A4 and resid 196 and name O)	5.16	0.09	0.09
40	assign (segid 3A4 and resid 193 and name CA) (segid 3A4 and resid 197 and name C)	4.54	0.09	0.10
	assign (segid 3A4 and resid 193 and name CA) (segid 3A4 and resid 197 and name CB)	4.56	0.08	0.09
	assign (segid 3A4 and resid 193 and name CA) (segid 3A4 and resid 197 and name N)	6.97	0.05	0.05
	assign (segid 3A4 and resid 193 and name CA) (segid 3A4 and resid 197 and name O)	7.43	0.09	0.10
45	assign (segid 3A4 and resid 193 and name CA) (segid 3A4 and resid 198 and name C)	6.25	0.08	0.08
	assign (segid 3A4 and resid 193 and name CA) (segid 3A4 and resid 198 and name CB)	5.91	0.08	0.07
	assign (segid 3A4 and resid 193 and name CA) (segid 3A4 and resid 198 and name N)	7.24	0.10	0.10
	assign (segid 3A4 and resid 193 and name CA) (segid 3A4 and resid 198 and name O)	8.71	0.11	0.11
50	assign (segid 3A4 and resid 193 and name CA) (segid 3A4 and resid 199 and name C)	8.76	0.10	0.10
	assign (segid 3A4 and resid 193 and name CA) (segid 3A4 and resid 199 and name CB)	7.40	0.11	0.11
	assign (segid 3A4 and resid 193 and name CA) (segid 3A4 and resid 199 and name N)	9.97	0.08	0.09
	assign (segid 3A4 and resid 193 and name CA) (segid 3A4 and resid 199 and name O)	9.46	0.14	0.14
55	assign (segid 3A4 and resid 193 and name CA) (segid 3A4 and resid 200 and name C)	11.15	0.45	0.45
	assign (segid 3A4 and resid 193 and name CA) (segid 3A4 and resid 200 and name CB)	12.84	0.39	0.39
	assign (segid 3A4 and resid 193 and name CA) (segid 3A4 and resid 200 and name N)	12.42	0.44	0.43
	assign (segid 3A4 and resid 193 and name CA) (segid 3A4 and resid 200 and name O)	14.51	0.16	0.15
60	assign (segid 3A4 and resid 193 and name CA) (segid 3A4 and resid 201 and name C)	14.01	0.12	0.12
	assign (segid 3A4 and resid 193 and name CA) (segid 3A4 and resid 201 and name CB)	15.81	0.25	0.24
	assign (segid 3A4 and resid 193 and name CA) (segid 3A4 and resid 201 and name N)	15.16	0.33	0.34
	assign (segid 3A4 and resid 193 and name CA) (segid 3A4 and resid 201 and name O)	17.16	0.37	0.37
65	assign (segid 3A4 and resid 193 and name CA) (segid 3A4 and resid 202 and name C)	16.52	0.35	0.36
	assign (segid 3A4 and resid 193 and name CA) (segid 3A4 and resid 202 and name CB)	18.69	0.32	0.32
	assign (segid 3A4 and resid 193 and name CA) (segid 3A4 and resid 202 and name N)	18.09	0.34	0.34
	assign (segid 3A4 and resid 193 and name CA) (segid 3A4 and resid 202 and name O)	18.11	0.59	0.59
70	assign (segid 3A4 and resid 193 and name CA) (segid 3A4 and resid 203 and name C)	16.98	0.57	0.58
	assign (segid 3A4 and resid 193 and name CA) (segid 3A4 and resid 203 and name CB)	16.44	1.18	1.19
	assign (segid 3A4 and resid 193 and name CA) (segid 3A4 and resid 203 and name N)	16.16	1.41	1.41
	assign (segid 3A4 and resid 193 and name CA) (segid 3A4 and resid 203 and name O)	14.80	0.82	0.81
75	assign (segid 3A4 and resid 193 and name CA) (segid 3A4 and resid 204 and name C)	15.30	0.80	0.80
	assign (segid 3A4 and resid 193 and name CA) (segid 3A4 and resid 204 and name CB)	16.79	0.60	0.61
	assign (segid 3A4 and resid 193 and name CA) (segid 3A4 and resid 204 and name N)	18.31	0.61	0.61
	assign (segid 3A4 and resid 193 and name CA) (segid 3A4 and resid 204 and name O)	16.06	0.65	0.65
80	assign (segid 3A4 and resid 193 and name CA) (segid 3A4 and resid 205 and name C)	16.35	0.82	0.81
	assign (segid 3A4 and resid 193 and name CA) (segid 3A4 and resid 205 and name CB)	12.33	0.63	0.62
	assign (segid 3A4 and resid 193 and name CA) (segid 3A4 and resid 205 and name N)	11.50	0.78	0.78
	assign (segid 3A4 and resid 193 and name CA) (segid 3A4 and resid 205 and name O)	13.20	0.31	0.30
	assign (segid 3A4 and resid 193 and name CA) (segid 3A4 and resid 206 and name C)	14.08	0.33	0.33
	assign (segid 3A4 and resid 193 and name CA) (segid 3A4 and resid 206 and name CB)	15.70	0.31	0.32
	assign (segid 3A4 and resid 193 and name CA) (segid 3A4 and resid 206 and name N)	16.86	0.37	0.37
	assign (segid 3A4 and resid 193 and name CA) (segid 3A4 and resid 206 and name O)	13.70	0.33	0.32
	assign (segid 3A4 and resid 193 and name CA) (segid 3A4 and resid 207 and name C)	13.10	0.40	0.39
	assign (segid 3A4 and resid 193 and name CA) (segid 3A4 and resid 207 and name CB)	11.33	0.53	0.52
	assign (segid 3A4 and resid 193 and name CA) (segid 3A4 and resid 207 and name N)	14.54	0.69	0.69

	assign (segid 3A4 and resid 193 and name CA)	(segid 3A4 and resid 250 and name CB)	15.58	0.60	0.59
	assign (segid 3A4 and resid 193 and name CA)	(segid 3A4 and resid 251 and name CA)	16.23	0.69	0.69
	assign (segid 3A4 and resid 193 and name CA)	(segid 3A4 and resid 251 and name CB)	16.62	0.59	0.59
	assign (segid 3A4 and resid 193 and name CA)	(segid 3A4 and resid 252 and name CA)	13.84	0.94	0.94
5	assign (segid 3A4 and resid 193 and name CA)	(segid 3A4 and resid 252 and name CB)	12.43	0.94	0.94
	assign (segid 3A4 and resid 193 and name CA)	(segid 3A4 and resid 253 and name CA)	13.85	1.07	1.07
	assign (segid 3A4 and resid 193 and name CA)	(segid 3A4 and resid 254 and name CA)	17.47	0.99	1.00
	assign (segid 3A4 and resid 193 and name CB)	(segid 3A4 and resid 194 and name C)	5.39	0.06	0.06
	assign (segid 3A4 and resid 193 and name CB)	(segid 3A4 and resid 194 and name CB)	4.46	0.06	0.06
10	assign (segid 3A4 and resid 193 and name CB)	(segid 3A4 and resid 194 and name N)	5.33	0.06	0.07
	assign (segid 3A4 and resid 193 and name CB)	(segid 3A4 and resid 194 and name O)	3.12	0.06	0.06
	assign (segid 3A4 and resid 193 and name CB)	(segid 3A4 and resid 194 and name O)	6.20	0.17	0.17
	assign (segid 3A4 and resid 193 and name CB)	(segid 3A4 and resid 195 and name C)	6.92	0.07	0.07
	assign (segid 3A4 and resid 193 and name CB)	(segid 3A4 and resid 195 and name CB)	6.78	0.06	0.06
15	assign (segid 3A4 and resid 193 and name CB)	(segid 3A4 and resid 195 and name N)	7.27	0.06	0.06
	assign (segid 3A4 and resid 193 and name CB)	(segid 3A4 and resid 195 and name N)	5.59	0.06	0.06
	assign (segid 3A4 and resid 193 and name CB)	(segid 3A4 and resid 196 and name C)	6.99	0.06	0.06
	assign (segid 3A4 and resid 193 and name CB)	(segid 3A4 and resid 196 and name CA)	6.54	0.11	0.11
	assign (segid 3A4 and resid 193 and name CB)	(segid 3A4 and resid 196 and name CB)	5.84	0.14	0.14
20	assign (segid 3A4 and resid 193 and name CB)	(segid 3A4 and resid 196 and name N)	6.02	0.10	0.09
	assign (segid 3A4 and resid 193 and name CB)	(segid 3A4 and resid 197 and name CA)	7.10	0.15	0.14
	assign (segid 3A4 and resid 193 and name CB)	(segid 3A4 and resid 197 and name CB)	6.50	0.16	0.15
	assign (segid 3A4 and resid 193 and name CB)	(segid 3A4 and resid 197 and name CG)	7.66	0.20	0.20
	assign (segid 3A4 and resid 193 and name CB)	(segid 3A4 and resid 197 and name N)	6.30	0.11	0.11
25	assign (segid 3A4 and resid 193 and name CB)	(segid 3A4 and resid 198 and name CA)	9.75	0.17	0.17
	assign (segid 3A4 and resid 193 and name CB)	(segid 3A4 and resid 198 and name CB)	9.81	0.15	0.15
	assign (segid 3A4 and resid 193 and name CB)	(segid 3A4 and resid 199 and name CA)	11.30	0.11	0.11
	assign (segid 3A4 and resid 193 and name CB)	(segid 3A4 and resid 199 and name CB)	10.87	0.15	0.14
	assign (segid 3A4 and resid 193 and name CB)	(segid 3A4 and resid 200 and name CA)	12.25	0.51	0.51
30	assign (segid 3A4 and resid 193 and name CB)	(segid 3A4 and resid 201 and name CA)	13.78	0.47	0.47
	assign (segid 3A4 and resid 193 and name CB)	(segid 3A4 and resid 201 and name CB)	13.28	0.50	0.50
	assign (segid 3A4 and resid 193 and name CB)	(segid 3A4 and resid 202 and name CA)	15.67	0.22	0.22
	assign (segid 3A4 and resid 193 and name CB)	(segid 3A4 and resid 202 and name CB)	15.24	0.14	0.15
	assign (segid 3A4 and resid 193 and name CB)	(segid 3A4 and resid 203 and name CA)	17.03	0.31	0.31
35	assign (segid 3A4 and resid 193 and name CB)	(segid 3A4 and resid 203 and name CB)	16.40	0.38	0.37
	assign (segid 3A4 and resid 193 and name CB)	(segid 3A4 and resid 204 and name CA)	18.17	0.44	0.45
	assign (segid 3A4 and resid 193 and name CB)	(segid 3A4 and resid 204 and name CB)	17.44	0.43	0.43
	assign (segid 3A4 and resid 193 and name CB)	(segid 3A4 and resid 205 and name CB)	19.09	0.43	0.44
	assign (segid 3A4 and resid 193 and name CB)	(segid 3A4 and resid 221 and name CB)	17.86	0.51	0.50
40	assign (segid 3A4 and resid 193 and name CB)	(segid 3A4 and resid 241 and name CA)	17.86	1.16	1.17
	assign (segid 3A4 and resid 193 and name CB)	(segid 3A4 and resid 241 and name CB)	17.61	1.40	1.40
	assign (segid 3A4 and resid 193 and name CB)	(segid 3A4 and resid 242 and name CA)	16.19	0.82	0.83
	assign (segid 3A4 and resid 193 and name CB)	(segid 3A4 and resid 242 and name CB)	16.70	0.82	0.81
	assign (segid 3A4 and resid 193 and name CB)	(segid 3A4 and resid 243 and name CA)	18.05	0.59	0.60
45	assign (segid 3A4 and resid 193 and name CB)	(segid 3A4 and resid 244 and name CA)	17.27	0.62	0.62
	assign (segid 3A4 and resid 193 and name CB)	(segid 3A4 and resid 244 and name CB)	17.59	0.78	0.78
	assign (segid 3A4 and resid 193 and name CB)	(segid 3A4 and resid 245 and name CA)	13.54	0.63	0.62
	assign (segid 3A4 and resid 193 and name CB)	(segid 3A4 and resid 245 and name CB)	12.80	0.80	0.79
	assign (segid 3A4 and resid 193 and name CB)	(segid 3A4 and resid 246 and name CA)	14.25	0.31	0.31
50	assign (segid 3A4 and resid 193 and name CB)	(segid 3A4 and resid 246 and name CB)	15.16	0.34	0.34
	assign (segid 3A4 and resid 193 and name CB)	(segid 3A4 and resid 247 and name CA)	16.62	0.31	0.31
	assign (segid 3A4 and resid 193 and name CB)	(segid 3A4 and resid 247 and name CB)	17.81	0.35	0.36
	assign (segid 3A4 and resid 193 and name CB)	(segid 3A4 and resid 248 and name CA)	14.50	0.34	0.35
	assign (segid 3A4 and resid 193 and name CB)	(segid 3A4 and resid 248 and name CB)	13.96	0.43	0.43
55	assign (segid 3A4 and resid 193 and name CB)	(segid 3A4 and resid 249 and name CA)	11.98	0.50	0.50
	assign (segid 3A4 and resid 193 and name CB)	(segid 3A4 and resid 250 and name CA)	15.06	0.69	0.69
	assign (segid 3A4 and resid 193 and name CB)	(segid 3A4 and resid 250 and name CB)	16.18	0.61	0.61
	assign (segid 3A4 and resid 193 and name CB)	(segid 3A4 and resid 251 and name CA)	16.66	0.72	0.71
	assign (segid 3A4 and resid 193 and name CB)	(segid 3A4 and resid 251 and name CB)	17.11	0.62	0.62
60	assign (segid 3A4 and resid 193 and name CB)	(segid 3A4 and resid 252 and name CA)	14.02	0.97	0.96
	assign (segid 3A4 and resid 193 and name CB)	(segid 3A4 and resid 252 and name CB)	12.63	0.96	0.96
	assign (segid 3A4 and resid 193 and name CB)	(segid 3A4 and resid 253 and name CA)	13.85	1.09	1.08
	assign (segid 3A4 and resid 193 and name N)	(segid 3A4 and resid 193 and name C)	2.45	0.02	0.02
65	assign (segid 3A4 and resid 193 and name N)	(segid 3A4 and resid 193 and name CA)	1.46	0.01	0.01
	assign (segid 3A4 and resid 193 and name N)	(segid 3A4 and resid 193 and name CB)	2.46	0.04	0.04
	assign (segid 3A4 and resid 193 and name N)	(segid 3A4 and resid 193 and name O)	3.48	0.03	0.03
	assign (segid 3A4 and resid 193 and name N)	(segid 3A4 and resid 194 and name C)	4.63	0.03	0.03
	assign (segid 3A4 and resid 193 and name N)	(segid 3A4 and resid 194 and name CA)	4.21	0.02	0.03
	assign (segid 3A4 and resid 193 and name N)	(segid 3A4 and resid 194 and name CB)	5.01	0.06	0.07
70	assign (segid 3A4 and resid 193 and name N)	(segid 3A4 and resid 194 and name N)	2.82	0.03	0.03
	assign (segid 3A4 and resid 193 and name N)	(segid 3A4 and resid 194 and name O)	5.64	0.11	0.10
	assign (segid 3A4 and resid 193 and name N)	(segid 3A4 and resid 195 and name C)	5.52	0.09	0.09
	assign (segid 3A4 and resid 193 and name N)	(segid 3A4 and resid 195 and name CA)	5.21	0.09	0.08
	assign (segid 3A4 and resid 193 and name N)	(segid 3A4 and resid 195 and name CB)	5.28	0.06	0.07
75	assign (segid 3A4 and resid 193 and name N)	(segid 3A4 and resid 195 and name N)	4.25	0.09	0.08
	assign (segid 3A4 and resid 193 and name N)	(segid 3A4 and resid 195 and name O)	6.73	0.09	0.08
	assign (segid 3A4 and resid 193 and name N)	(segid 3A4 and resid 196 and name C)	6.43	0.10	0.09
	assign (segid 3A4 and resid 193 and name N)	(segid 3A4 and resid 196 and name CA)	5.54	0.11	0.10
	assign (segid 3A4 and resid 193 and name N)	(segid 3A4 and resid 196 and name CB)	5.02	0.12	0.13
80	assign (segid 3A4 and resid 193 and name N)	(segid 3A4 and resid 196 and name N)	4.72	0.09	0.09
	assign (segid 3A4 and resid 193 and name N)	(segid 3A4 and resid 196 and name O)	7.62	0.09	0.10
	assign (segid 3A4 and resid 193 and name N)	(segid 3A4 and resid 197 and name CA)	7.23	0.08	0.08
	assign (segid 3A4 and resid 193 and name N)	(segid 3A4 and resid 197 and name CB)	7.00	0.06	0.07

	assign (segid 3A4 and resid 193 and name N)	(segid 3A4 and resid 197 and name N)	6.08	0.09	0.09
	assign (segid 3A4 and resid 193 and name O)	(segid 3A4 and resid 193 and name CB)	3.30	0.03	0.04
	assign (segid 3A4 and resid 193 and name O)	(segid 3A4 and resid 194 and name C)	2.98	0.09	0.09
	assign (segid 3A4 and resid 193 and name O)	(segid 3A4 and resid 194 and name CA)	2.78	0.03	0.03
5	assign (segid 3A4 and resid 193 and name O)	(segid 3A4 and resid 194 and name CB)	4.28	0.02	0.02
	assign (segid 3A4 and resid 193 and name O)	(segid 3A4 and resid 194 and name N)	2.27	0.02	0.01
	assign (segid 3A4 and resid 193 and name O)	(segid 3A4 and resid 194 and name O)	3.34	0.22	0.22
	assign (segid 3A4 and resid 193 and name O)	(segid 3A4 and resid 195 and name C)	4.22	0.10	0.11
	assign (segid 3A4 and resid 193 and name O)	(segid 3A4 and resid 195 and name CA)	4.48	0.09	0.08
	assign (segid 3A4 and resid 193 and name O)	(segid 3A4 and resid 195 and name CB)	5.48	0.12	0.11
10	assign (segid 3A4 and resid 193 and name O)	(segid 3A4 and resid 195 and name N)	3.53	0.08	0.08
	assign (segid 3A4 and resid 193 and name O)	(segid 3A4 and resid 195 and name O)	5.14	0.07	0.07
	assign (segid 3A4 and resid 193 and name O)	(segid 3A4 and resid 196 and name C)	3.94	0.10	0.10
	assign (segid 3A4 and resid 193 and name O)	(segid 3A4 and resid 196 and name CA)	3.86	0.14	0.15
	assign (segid 3A4 and resid 193 and name O)	(segid 3A4 and resid 196 and name CB)	3.72	0.17	0.16
15	assign (segid 3A4 and resid 193 and name O)	(segid 3A4 and resid 196 and name N)	3.40	0.15	0.16
	assign (segid 3A4 and resid 193 and name O)	(segid 3A4 and resid 196 and name O)	5.11	0.09	0.10
	assign (segid 3A4 and resid 193 and name O)	(segid 3A4 and resid 197 and name C)	5.12	0.12	0.12
	assign (segid 3A4 and resid 193 and name O)	(segid 3A4 and resid 197 and name CA)	3.95	0.09	0.08
	assign (segid 3A4 and resid 193 and name O)	(segid 3A4 and resid 197 and name CB)	3.58	0.06	0.06
20	assign (segid 3A4 and resid 193 and name O)	(segid 3A4 and resid 197 and name CG)	4.98	0.07	0.07
	assign (segid 3A4 and resid 193 and name O)	(segid 3A4 and resid 197 and name N)	3.10	0.11	0.10
	assign (segid 3A4 and resid 193 and name O)	(segid 3A4 and resid 197 and name O)	6.25	0.11	0.11
	assign (segid 3A4 and resid 193 and name O)	(segid 3A4 and resid 198 and name C)	7.41	0.19	0.19
	assign (segid 3A4 and resid 193 and name O)	(segid 3A4 and resid 198 and name CA)	6.53	0.18	0.18
25	assign (segid 3A4 and resid 193 and name O)	(segid 3A4 and resid 198 and name CB)	6.76	0.18	0.18
	assign (segid 3A4 and resid 193 and name O)	(segid 3A4 and resid 198 and name CG)	6.62	0.29	0.30
	assign (segid 3A4 and resid 193 and name O)	(segid 3A4 and resid 198 and name N)	5.16	0.17	0.18
	assign (segid 3A4 and resid 193 and name O)	(segid 3A4 and resid 199 and name N)	7.08	0.18	0.18
	assign (segid 3A4 and resid 193 and name O)	(segid 3A4 and resid 194 and name CB)	2.52	0.04	0.03
30	assign (segid 3A4 and resid 194 and name C)	(segid 3A4 and resid 194 and name O)	1.23	0.01	0.00
	assign (segid 3A4 and resid 194 and name C)	(segid 3A4 and resid 195 and name C)	3.02	0.03	0.03
	assign (segid 3A4 and resid 194 and name C)	(segid 3A4 and resid 195 and name CA)	2.44	0.02	0.01
	assign (segid 3A4 and resid 194 and name C)	(segid 3A4 and resid 195 and name CB)	3.71	0.03	0.02
	assign (segid 3A4 and resid 194 and name C)	(segid 3A4 and resid 195 and name N)	1.33	0.01	0.00
35	assign (segid 3A4 and resid 194 and name C)	(segid 3A4 and resid 195 and name O)	3.85	0.03	0.03
	assign (segid 3A4 and resid 194 and name C)	(segid 3A4 and resid 196 and name C)	4.51	0.11	0.11
	assign (segid 3A4 and resid 194 and name C)	(segid 3A4 and resid 196 and name CA)	4.43	0.10	0.10
	assign (segid 3A4 and resid 194 and name C)	(segid 3A4 and resid 196 and name CB)	5.17	0.10	0.11
	assign (segid 3A4 and resid 194 and name C)	(segid 3A4 and resid 196 and name N)	3.25	0.09	0.10
40	assign (segid 3A4 and resid 194 and name C)	(segid 3A4 and resid 196 and name O)	5.53	0.19	0.19
	assign (segid 3A4 and resid 194 and name C)	(segid 3A4 and resid 197 and name C)	4.89	0.08	0.08
	assign (segid 3A4 and resid 194 and name C)	(segid 3A4 and resid 197 and name CA)	4.54	0.15	0.14
	assign (segid 3A4 and resid 194 and name C)	(segid 3A4 and resid 197 and name CB)	4.25	0.27	0.27
	assign (segid 3A4 and resid 194 and name C)	(segid 3A4 and resid 197 and name CG)	5.43	0.32	0.31
45	assign (segid 3A4 and resid 194 and name C)	(segid 3A4 and resid 197 and name N)	3.84	0.08	0.07
	assign (segid 3A4 and resid 194 and name C)	(segid 3A4 and resid 197 and name O)	6.12	0.07	0.07
	assign (segid 3A4 and resid 194 and name C)	(segid 3A4 and resid 198 and name C)	6.14	0.04	0.05
	assign (segid 3A4 and resid 194 and name C)	(segid 3A4 and resid 198 and name CA)	5.10	0.06	0.06
	assign (segid 3A4 and resid 194 and name C)	(segid 3A4 and resid 198 and name CB)	4.69	0.08	0.08
50	assign (segid 3A4 and resid 194 and name C)	(segid 3A4 and resid 198 and name CG)	4.40	0.19	0.19
	assign (segid 3A4 and resid 194 and name C)	(segid 3A4 and resid 198 and name N)	4.18	0.05	0.05
	assign (segid 3A4 and resid 194 and name C)	(segid 3A4 and resid 198 and name O)	7.32	0.05	0.06
	assign (segid 3A4 and resid 194 and name C)	(segid 3A4 and resid 199 and name C)	7.18	0.10	0.10
	assign (segid 3A4 and resid 194 and name C)	(segid 3A4 and resid 199 and name CB)	7.12	0.17	0.18
55	assign (segid 3A4 and resid 194 and name C)	(segid 3A4 and resid 199 and name N)	5.94	0.07	0.07
	assign (segid 3A4 and resid 194 and name CA)	(segid 3A4 and resid 194 and name C)	1.53	0.01	0.01
	assign (segid 3A4 and resid 194 and name CA)	(segid 3A4 and resid 194 and name CB)	1.54	0.01	0.02
	assign (segid 3A4 and resid 194 and name CA)	(segid 3A4 and resid 194 and name O)	2.40	0.01	0.01
	assign (segid 3A4 and resid 194 and name CA)	(segid 3A4 and resid 195 and name C)	4.43	0.01	0.01
60	assign (segid 3A4 and resid 194 and name CA)	(segid 3A4 and resid 195 and name CA)	3.80	0.02	0.02
	assign (segid 3A4 and resid 194 and name CA)	(segid 3A4 and resid 195 and name CB)	4.85	0.02	0.03
	assign (segid 3A4 and resid 194 and name CA)	(segid 3A4 and resid 195 and name N)	2.42	0.02	0.02
	assign (segid 3A4 and resid 194 and name CA)	(segid 3A4 and resid 195 and name O)	5.33	0.04	0.04
	assign (segid 3A4 and resid 194 and name CA)	(segid 3A4 and resid 196 and name C)	5.51	0.09	0.09
65	assign (segid 3A4 and resid 194 and name CA)	(segid 3A4 and resid 196 and name CA)	5.46	0.06	0.07
	assign (segid 3A4 and resid 194 and name CA)	(segid 3A4 and resid 196 and name CB)	5.88	0.07	0.08
	assign (segid 3A4 and resid 194 and name CA)	(segid 3A4 and resid 196 and name N)	4.39	0.06	0.06
	assign (segid 3A4 and resid 194 and name CA)	(segid 3A4 and resid 196 and name O)	6.60	0.15	0.15
	assign (segid 3A4 and resid 194 and name CA)	(segid 3A4 and resid 197 and name C)	5.78	0.09	0.09
70	assign (segid 3A4 and resid 194 and name CA)	(segid 3A4 and resid 197 and name CA)	5.17	0.15	0.16
	assign (segid 3A4 and resid 194 and name CA)	(segid 3A4 and resid 197 and name CB)	4.47	0.28	0.29
	assign (segid 3A4 and resid 194 and name CA)	(segid 3A4 and resid 197 and name CG)	5.54	0.34	0.35
	assign (segid 3A4 and resid 194 and name CA)	(segid 3A4 and resid 197 and name N)	4.63	0.10	0.09
	assign (segid 3A4 and resid 194 and name CA)	(segid 3A4 and resid 197 and name O)	6.98	0.10	0.10
75	assign (segid 3A4 and resid 194 and name CA)	(segid 3A4 and resid 198 and name C)	7.43	0.08	0.07
	assign (segid 3A4 and resid 194 and name CA)	(segid 3A4 and resid 198 and name CA)	6.25	0.08	0.08
	assign (segid 3A4 and resid 194 and name CA)	(segid 3A4 and resid 198 and name CB)	5.88	0.08	0.08
	assign (segid 3A4 and resid 194 and name CA)	(segid 3A4 and resid 198 and name CG)	5.30	0.20	0.19
	assign (segid 3A4 and resid 194 and name CA)	(segid 3A4 and resid 198 and name N)	5.25	0.08	0.08
80	assign (segid 3A4 and resid 194 and name CA)	(segid 3A4 and resid 199 and name CA)	8.60	0.11	0.11
	assign (segid 3A4 and resid 194 and name CA)	(segid 3A4 and resid 199 and name CB)	8.56	0.17	0.18
	assign (segid 3A4 and resid 194 and name CA)	(segid 3A4 and resid 199 and name N)	7.33	0.10	0.09

	assign (segid 3A4 and resid 194 and name CA) (segid 3A4 and resid 200 and name CA)	10.31	0.35	0.35
	assign (segid 3A4 and resid 194 and name CA) (segid 3A4 and resid 201 and name CA)	10.99	0.35	0.34
	assign (segid 3A4 and resid 194 and name CA) (segid 3A4 and resid 201 and name CB)	10.22	0.43	0.44
	assign (segid 3A4 and resid 194 and name CA) (segid 3A4 and resid 202 and name CA)	12.43	0.16	0.16
	assign (segid 3A4 and resid 194 and name CA) (segid 3A4 and resid 202 and name CB)	11.90	0.15	0.15
5	assign (segid 3A4 and resid 194 and name CA) (segid 3A4 and resid 203 and name CA)	14.53	0.15	0.15
	assign (segid 3A4 and resid 194 and name CA) (segid 3A4 and resid 203 and name CB)	14.23	0.21	0.22
	assign (segid 3A4 and resid 194 and name CA) (segid 3A4 and resid 204 and name CA)	15.81	0.23	0.24
	assign (segid 3A4 and resid 194 and name CA) (segid 3A4 and resid 204 and name CB)	15.20	0.26	0.26
	assign (segid 3A4 and resid 194 and name CA) (segid 3A4 and resid 205 and name CA)	16.65	0.26	0.26
10	assign (segid 3A4 and resid 194 and name CA) (segid 3A4 and resid 205 and name CB)	15.81	0.31	0.31
	assign (segid 3A4 and resid 194 and name CA) (segid 3A4 and resid 206 and name CA)	18.61	0.19	0.18
	assign (segid 3A4 and resid 194 and name CA) (segid 3A4 and resid 206 and name CB)	18.22	0.17	0.17
	assign (segid 3A4 and resid 194 and name CA) (segid 3A4 and resid 219 and name CA)	18.59	0.57	0.58
	assign (segid 3A4 and resid 194 and name CA) (segid 3A4 and resid 219 and name CB)	17.55	0.58	0.58
15	assign (segid 3A4 and resid 194 and name CA) (segid 3A4 and resid 220 and name CA)	17.05	0.68	0.69
	assign (segid 3A4 and resid 194 and name CA) (segid 3A4 and resid 220 and name CB)	16.34	0.79	0.79
	assign (segid 3A4 and resid 194 and name CA) (segid 3A4 and resid 221 and name CA)	14.94	0.63	0.63
	assign (segid 3A4 and resid 194 and name CA) (segid 3A4 and resid 221 and name CB)	13.91	0.64	0.64
	assign (segid 3A4 and resid 194 and name CA) (segid 3A4 and resid 222 and name CA)	18.18	0.66	0.65
20	assign (segid 3A4 and resid 194 and name CA) (segid 3A4 and resid 224 and name CA)	17.94	0.77	0.78
	assign (segid 3A4 and resid 194 and name CA) (segid 3A4 and resid 224 and name CB)	16.60	0.73	0.73
	assign (segid 3A4 and resid 194 and name CA) (segid 3A4 and resid 225 and name CA)	18.02	1.11	1.10
	assign (segid 3A4 and resid 194 and name CA) (segid 3A4 and resid 225 and name CB)	17.62	1.14	1.13
	assign (segid 3A4 and resid 194 and name CA) (segid 3A4 and resid 240 and name CA)	17.70	0.84	0.84
25	assign (segid 3A4 and resid 194 and name CA) (segid 3A4 and resid 240 and name CB)	17.89	0.79	0.79
	assign (segid 3A4 and resid 194 and name CA) (segid 3A4 and resid 241 and name CA)	14.59	1.03	1.03
	assign (segid 3A4 and resid 194 and name CA) (segid 3A4 and resid 241 and name CB)	14.60	1.23	1.23
	assign (segid 3A4 and resid 194 and name CA) (segid 3A4 and resid 242 and name CA)	12.99	0.73	0.72
	assign (segid 3A4 and resid 194 and name CA) (segid 3A4 and resid 242 and name CB)	13.73	0.70	0.70
30	assign (segid 3A4 and resid 194 and name CA) (segid 3A4 and resid 243 and name CA)	14.31	0.58	0.58
	assign (segid 3A4 and resid 194 and name CA) (segid 3A4 and resid 243 and name CB)	15.80	0.57	0.57
	assign (segid 3A4 and resid 194 and name CA) (segid 3A4 and resid 244 and name CA)	13.24	0.60	0.59
	assign (segid 3A4 and resid 194 and name CA) (segid 3A4 and resid 244 and name CB)	13.64	0.75	0.76
	assign (segid 3A4 and resid 194 and name CA) (segid 3A4 and resid 245 and name CA)	9.56	0.67	0.66
35	assign (segid 3A4 and resid 194 and name CA) (segid 3A4 and resid 245 and name CB)	9.08	0.84	0.84
	assign (segid 3A4 and resid 194 and name CA) (segid 3A4 and resid 246 and name CA)	10.29	0.35	0.35
	assign (segid 3A4 and resid 194 and name CA) (segid 3A4 and resid 246 and name CB)	11.38	0.38	0.39
	assign (segid 3A4 and resid 194 and name CA) (segid 3A4 and resid 247 and name CA)	12.32	0.33	0.33
	assign (segid 3A4 and resid 194 and name CA) (segid 3A4 and resid 247 and name CB)	13.49	0.38	0.37
40	assign (segid 3A4 and resid 194 and name CA) (segid 3A4 and resid 248 and name CA)	10.09	0.35	0.36
	assign (segid 3A4 and resid 194 and name CA) (segid 3A4 and resid 248 and name CB)	9.59	0.45	0.46
	assign (segid 3A4 and resid 194 and name CA) (segid 3A4 and resid 249 and name CA)	7.72	0.51	0.51
	assign (segid 3A4 and resid 194 and name CA) (segid 3A4 and resid 250 and name CA)	11.02	0.69	0.69
	assign (segid 3A4 and resid 194 and name CA) (segid 3A4 and resid 250 and name CB)	12.13	0.59	0.60
45	assign (segid 3A4 and resid 194 and name CA) (segid 3A4 and resid 251 and name CA)	12.48	0.68	0.69
	assign (segid 3A4 and resid 194 and name CA) (segid 3A4 and resid 251 and name CB)	12.85	0.59	0.60
	assign (segid 3A4 and resid 194 and name CA) (segid 3A4 and resid 252 and name CA)	10.18	0.93	0.94
	assign (segid 3A4 and resid 194 and name CA) (segid 3A4 and resid 252 and name CB)	8.76	0.94	0.95
	assign (segid 3A4 and resid 194 and name CA) (segid 3A4 and resid 253 and name CA)	10.53	1.04	1.04
50	assign (segid 3A4 and resid 194 and name CA) (segid 3A4 and resid 254 and name CA)	14.08	0.96	0.96
	assign (segid 3A4 and resid 194 and name CA) (segid 3A4 and resid 255 and name CA)	15.13	1.09	1.08
	assign (segid 3A4 and resid 194 and name CA) (segid 3A4 and resid 256 and name CA)	14.31	1.21	1.21
	assign (segid 3A4 and resid 194 and name CA) (segid 3A4 and resid 257 and name CA)	15.67	1.54	1.54
	assign (segid 3A4 and resid 194 and name CB) (segid 3A4 and resid 195 and name C)	5.42	0.08	0.07
55	assign (segid 3A4 and resid 194 and name CB) (segid 3A4 and resid 195 and name CA)	4.44	0.09	0.09
	assign (segid 3A4 and resid 194 and name CB) (segid 3A4 and resid 195 and name CB)	5.29	0.11	0.11
	assign (segid 3A4 and resid 194 and name CB) (segid 3A4 and resid 195 and name N)	3.11	0.11	0.10
	assign (segid 3A4 and resid 194 and name CB) (segid 3A4 and resid 195 and name O)	6.27	0.06	0.07
	assign (segid 3A4 and resid 194 and name CB) (segid 3A4 and resid 196 and name C)	6.91	0.10	0.09
60	assign (segid 3A4 and resid 194 and name CB) (segid 3A4 and resid 196 and name CA)	6.82	0.07	0.07
	assign (segid 3A4 and resid 194 and name CB) (segid 3A4 and resid 196 and name CB)	7.32	0.07	0.06
	assign (segid 3A4 and resid 194 and name CB) (segid 3A4 and resid 196 and name N)	5.62	0.09	0.08
	assign (segid 3A4 and resid 194 and name CB) (segid 3A4 and resid 197 and name C)	6.92	0.13	0.12
	assign (segid 3A4 and resid 194 and name CB) (segid 3A4 and resid 197 and name CA)	6.50	0.18	0.19
65	assign (segid 3A4 and resid 194 and name CB) (segid 3A4 and resid 197 and name CB)	5.72	0.35	0.34
	assign (segid 3A4 and resid 194 and name CB) (segid 3A4 and resid 197 and name CG)	6.58	0.46	0.46
	assign (segid 3A4 and resid 194 and name CB) (segid 3A4 and resid 197 and name N)	6.05	0.08	0.09
	assign (segid 3A4 and resid 194 and name CB) (segid 3A4 and resid 198 and name CA)	6.99	0.08	0.08
	assign (segid 3A4 and resid 194 and name CB) (segid 3A4 and resid 198 and name CB)	6.33	0.05	0.05
70	assign (segid 3A4 and resid 194 and name CB) (segid 3A4 and resid 198 and name CG)	5.50	0.15	0.15
	assign (segid 3A4 and resid 194 and name CB) (segid 3A4 and resid 198 and name N)	6.21	0.08	0.09
	assign (segid 3A4 and resid 194 and name CB) (segid 3A4 and resid 199 and name CA)	9.53	0.14	0.14
	assign (segid 3A4 and resid 194 and name CB) (segid 3A4 and resid 199 and name CB)	9.55	0.21	0.22
	assign (segid 3A4 and resid 194 and name CB) (segid 3A4 and resid 200 and name CA)	11.49	0.31	0.31
75	assign (segid 3A4 and resid 194 and name CB) (segid 3A4 and resid 201 and name CA)	11.86	0.34	0.34
	assign (segid 3A4 and resid 194 and name CB) (segid 3A4 and resid 201 and name CB)	10.98	0.45	0.45
	assign (segid 3A4 and resid 194 and name CB) (segid 3A4 and resid 202 and name CA)	13.09	0.18	0.19
	assign (segid 3A4 and resid 194 and name CB) (segid 3A4 and resid 202 and name CB)	12.50	0.21	0.21
	assign (segid 3A4 and resid 194 and name CB) (segid 3A4 and resid 203 and name CA)	15.46	0.14	0.13
80	assign (segid 3A4 and resid 194 and name CB) (segid 3A4 and resid 203 and name CB)	15.26	0.19	0.19
	assign (segid 3A4 and resid 194 and name CB) (segid 3A4 and resid 204 and name CA)	16.78	0.21	0.21
	assign (segid 3A4 and resid 194 and name CB) (segid 3A4 and resid 204 and name CB)	16.19	0.27	0.27

	assign (segid 3A4 and resid 194 and name CB)	(segid 3A4 and resid 205 and name CA)	17.33	0.28	0.28
	assign (segid 3A4 and resid 194 and name CB)	(segid 3A4 and resid 205 and name CB)	16.39	0.32	0.33
	assign (segid 3A4 and resid 194 and name CB)	(segid 3A4 and resid 206 and name CA)	19.30	0.24	0.23
	assign (segid 3A4 and resid 194 and name CB)	(segid 3A4 and resid 206 and name CB)	18.93	0.22	0.23
	assign (segid 3A4 and resid 194 and name CB)	(segid 3A4 and resid 219 and name CA)	18.59	0.59	0.58
5	assign (segid 3A4 and resid 194 and name CB)	(segid 3A4 and resid 219 and name CB)	17.61	0.58	0.59
	assign (segid 3A4 and resid 194 and name CB)	(segid 3A4 and resid 220 and name CA)	16.84	0.70	0.70
	assign (segid 3A4 and resid 194 and name CB)	(segid 3A4 and resid 220 and name CB)	16.02	0.80	0.79
	assign (segid 3A4 and resid 194 and name CB)	(segid 3A4 and resid 221 and name CA)	14.98	0.66	0.67
	assign (segid 3A4 and resid 194 and name CB)	(segid 3A4 and resid 221 and name CB)	14.06	0.68	0.68
10	assign (segid 3A4 and resid 194 and name CB)	(segid 3A4 and resid 222 and name CA)	18.38	0.68	0.68
	assign (segid 3A4 and resid 194 and name CB)	(segid 3A4 and resid 224 and name CA)	17.84	0.82	0.81
	assign (segid 3A4 and resid 194 and name CB)	(segid 3A4 and resid 224 and name CB)	16.44	0.78	0.78
	assign (segid 3A4 and resid 194 and name CB)	(segid 3A4 and resid 225 and name CA)	18.21	1.13	1.14
	assign (segid 3A4 and resid 194 and name CB)	(segid 3A4 and resid 225 and name CB)	17.92	1.16	1.16
15	assign (segid 3A4 and resid 194 and name CB)	(segid 3A4 and resid 240 and name CA)	17.77	0.88	0.88
	assign (segid 3A4 and resid 194 and name CB)	(segid 3A4 and resid 240 and name CB)	17.92	0.85	0.84
	assign (segid 3A4 and resid 194 and name CB)	(segid 3A4 and resid 241 and name CA)	14.86	1.07	1.07
	assign (segid 3A4 and resid 194 and name CB)	(segid 3A4 and resid 241 and name CB)	15.01	1.25	1.25
	assign (segid 3A4 and resid 194 and name CB)	(segid 3A4 and resid 242 and name CA)	13.02	0.84	0.83
20	assign (segid 3A4 and resid 194 and name CB)	(segid 3A4 and resid 242 and name CB)	13.74	0.82	0.82
	assign (segid 3A4 and resid 194 and name CB)	(segid 3A4 and resid 243 and name CA)	14.00	0.67	0.68
	assign (segid 3A4 and resid 194 and name CB)	(segid 3A4 and resid 243 and name CB)	15.48	0.67	0.67
	assign (segid 3A4 and resid 194 and name CB)	(segid 3A4 and resid 244 and name CA)	13.09	0.67	0.66
	assign (segid 3A4 and resid 194 and name CB)	(segid 3A4 and resid 244 and name CB)	13.64	0.80	0.81
25	assign (segid 3A4 and resid 194 and name CB)	(segid 3A4 and resid 245 and name CA)	9.46	0.78	0.78
	assign (segid 3A4 and resid 194 and name CB)	(segid 3A4 and resid 245 and name CB)	9.12	0.97	0.97
	assign (segid 3A4 and resid 194 and name CB)	(segid 3A4 and resid 246 and name CA)	9.67	0.51	0.50
	assign (segid 3A4 and resid 194 and name CB)	(segid 3A4 and resid 246 and name CB)	10.75	0.54	0.54
	assign (segid 3A4 and resid 194 and name CB)	(segid 3A4 and resid 247 and name CA)	11.61	0.41	0.42
30	assign (segid 3A4 and resid 194 and name CB)	(segid 3A4 and resid 247 and name CB)	12.87	0.46	0.45
	assign (segid 3A4 and resid 194 and name CB)	(segid 3A4 and resid 248 and name CA)	9.56	0.44	0.43
	assign (segid 3A4 and resid 194 and name CB)	(segid 3A4 and resid 248 and name CB)	9.27	0.54	0.54
	assign (segid 3A4 and resid 194 and name CB)	(segid 3A4 and resid 249 and name CA)	6.80	0.51	0.50
	assign (segid 3A4 and resid 194 and name CB)	(segid 3A4 and resid 250 and name CA)	9.85	0.71	0.70
35	assign (segid 3A4 and resid 194 and name CB)	(segid 3A4 and resid 250 and name CB)	10.99	0.63	0.63
	assign (segid 3A4 and resid 194 and name CB)	(segid 3A4 and resid 251 and name CA)	11.48	0.72	0.72
	assign (segid 3A4 and resid 194 and name CB)	(segid 3A4 and resid 251 and name CB)	11.99	0.63	0.63
	assign (segid 3A4 and resid 194 and name CB)	(segid 3A4 and resid 252 and name CA)	9.19	0.96	0.96
	assign (segid 3A4 and resid 194 and name CB)	(segid 3A4 and resid 252 and name CB)	7.85	0.96	0.97
40	assign (segid 3A4 and resid 194 and name CB)	(segid 3A4 and resid 253 and name CA)	9.19	1.06	1.06
	assign (segid 3A4 and resid 194 and name CB)	(segid 3A4 and resid 254 and name CA)	12.75	1.00	0.99
	assign (segid 3A4 and resid 194 and name CB)	(segid 3A4 and resid 255 and name CA)	13.97	1.09	1.10
	assign (segid 3A4 and resid 194 and name CB)	(segid 3A4 and resid 256 and name CA)	13.21	1.22	1.22
	assign (segid 3A4 and resid 194 and name CB)	(segid 3A4 and resid 257 and name CA)	14.42	1.59	1.58
45	assign (segid 3A4 and resid 194 and name CB)	(segid 3A4 and resid 258 and name CB)	17.44	1.20	1.20
	assign (segid 3A4 and resid 194 and name CB)	(segid 3A4 and resid 194 and name C)	2.43	0.01	0.02
	assign (segid 3A4 and resid 194 and name N)	(segid 3A4 and resid 194 and name CA)	1.46	0.00	0.00
	assign (segid 3A4 and resid 194 and name N)	(segid 3A4 and resid 194 and name CB)	2.48	0.03	0.02
	assign (segid 3A4 and resid 194 and name N)	(segid 3A4 and resid 194 and name O)	3.44	0.07	0.07
50	assign (segid 3A4 and resid 194 and name N)	(segid 3A4 and resid 195 and name C)	4.70	0.04	0.05
	assign (segid 3A4 and resid 194 and name N)	(segid 3A4 and resid 195 and name CA)	4.18	0.05	0.06
	assign (segid 3A4 and resid 194 and name N)	(segid 3A4 and resid 195 and name CB)	4.95	0.04	0.03
	assign (segid 3A4 and resid 194 and name N)	(segid 3A4 and resid 195 and name N)	2.79	0.07	0.06
	assign (segid 3A4 and resid 194 and name N)	(segid 3A4 and resid 195 and name O)	5.79	0.06	0.06
55	assign (segid 3A4 and resid 194 and name N)	(segid 3A4 and resid 196 and name C)	5.66	0.05	0.05
	assign (segid 3A4 and resid 194 and name N)	(segid 3A4 and resid 196 and name CA)	5.34	0.07	0.06
	assign (segid 3A4 and resid 194 and name N)	(segid 3A4 and resid 196 and name CB)	5.41	0.08	0.07
	assign (segid 3A4 and resid 194 and name N)	(segid 3A4 and resid 196 and name N)	4.32	0.07	0.06
	assign (segid 3A4 and resid 194 and name N)	(segid 3A4 and resid 196 and name O)	6.85	0.08	0.08
60	assign (segid 3A4 and resid 194 and name N)	(segid 3A4 and resid 197 and name C)	6.53	0.06	0.06
	assign (segid 3A4 and resid 194 and name N)	(segid 3A4 and resid 197 and name CA)	5.67	0.08	0.08
	assign (segid 3A4 and resid 194 and name N)	(segid 3A4 and resid 197 and name CB)	5.07	0.18	0.18
	assign (segid 3A4 and resid 194 and name N)	(segid 3A4 and resid 197 and name CG)	6.29	0.23	0.22
	assign (segid 3A4 and resid 194 and name N)	(segid 3A4 and resid 197 and name N)	4.89	0.05	0.04
65	assign (segid 3A4 and resid 194 and name N)	(segid 3A4 and resid 197 and name O)	7.75	0.07	0.06
	assign (segid 3A4 and resid 194 and name N)	(segid 3A4 and resid 198 and name CA)	7.30	0.08	0.09
	assign (segid 3A4 and resid 194 and name N)	(segid 3A4 and resid 198 and name CB)	7.06	0.09	0.09
	assign (segid 3A4 and resid 194 and name N)	(segid 3A4 and resid 198 and name CG)	6.63	0.21	0.22
	assign (segid 3A4 and resid 194 and name N)	(segid 3A4 and resid 198 and name N)	6.17	0.08	0.08
70	assign (segid 3A4 and resid 194 and name N)	(segid 3A4 and resid 198 and name CB)	3.36	0.06	0.06
	assign (segid 3A4 and resid 194 and name O)	(segid 3A4 and resid 195 and name C)	2.93	0.12	0.11
	assign (segid 3A4 and resid 194 and name O)	(segid 3A4 and resid 195 and name CA)	2.77	0.04	0.03
	assign (segid 3A4 and resid 194 and name O)	(segid 3A4 and resid 195 and name CB)	4.23	0.03	0.04
	assign (segid 3A4 and resid 194 and name O)	(segid 3A4 and resid 195 and name N)	2.25	0.01	0.00
75	assign (segid 3A4 and resid 194 and name O)	(segid 3A4 and resid 195 and name O)	3.41	0.09	0.09
	assign (segid 3A4 and resid 194 and name O)	(segid 3A4 and resid 196 and name C)	3.95	0.26	0.25
	assign (segid 3A4 and resid 194 and name O)	(segid 3A4 and resid 196 and name CA)	4.24	0.24	0.24
	assign (segid 3A4 and resid 194 and name O)	(segid 3A4 and resid 196 and name CB)	5.19	0.26	0.25
	assign (segid 3A4 and resid 194 and name O)	(segid 3A4 and resid 196 and name N)	3.31	0.21	0.21
80	assign (segid 3A4 and resid 194 and name O)	(segid 3A4 and resid 196 and name O)	4.83	0.33	0.32
	assign (segid 3A4 and resid 194 and name O)	(segid 3A4 and resid 197 and name C)	3.79	0.05	0.05
	assign (segid 3A4 and resid 194 and name O)	(segid 3A4 and resid 197 and name CA)	3.66	0.11	0.11

	assign (segid 3A4 and resid 194 and name O) (segid 3A4 and resid 197 and name CB)	3.48	0.23	0.23
	assign (segid 3A4 and resid 194 and name O) (segid 3A4 and resid 197 and name CG)	4.55	0.28	0.29
	assign (segid 3A4 and resid 194 and name O) (segid 3A4 and resid 197 and name N)	3.21	0.12	0.12
	assign (segid 3A4 and resid 194 and name O) (segid 3A4 and resid 197 and name O)	4.99	0.04	0.05
	assign (segid 3A4 and resid 194 and name O) (segid 3A4 and resid 198 and name C)	5.05	0.07	0.07
5	assign (segid 3A4 and resid 194 and name O) (segid 3A4 and resid 198 and name CA)	3.93	0.07	0.08
	assign (segid 3A4 and resid 194 and name O) (segid 3A4 and resid 198 and name CB)	3.66	0.11	0.11
	assign (segid 3A4 and resid 194 and name O) (segid 3A4 and resid 198 and name CG)	3.44	0.21	0.21
	assign (segid 3A4 and resid 194 and name O) (segid 3A4 and resid 198 and name N)	3.00	0.06	0.06
	assign (segid 3A4 and resid 194 and name O) (segid 3A4 and resid 198 and name O)	6.20	0.07	0.07
10	assign (segid 3A4 and resid 194 and name O) (segid 3A4 and resid 199 and name C)	7.27	0.18	0.18
	assign (segid 3A4 and resid 194 and name O) (segid 3A4 and resid 199 and name CA)	6.32	0.15	0.14
	assign (segid 3A4 and resid 194 and name O) (segid 3A4 and resid 199 and name CB)	6.45	0.21	0.21
	assign (segid 3A4 and resid 194 and name O) (segid 3A4 and resid 199 and name N)	4.98	0.11	0.12
	assign (segid 3A4 and resid 194 and name O) (segid 3A4 and resid 200 and name N)	7.03	0.31	0.32
15	assign (segid 3A4 and resid 194 and name O) (segid 3A4 and resid 245 and name O)	7.20	0.18	0.19
	assign (segid 3A4 and resid 195 and name C) (segid 3A4 and resid 195 and name CB)	2.50	0.04	0.04
	assign (segid 3A4 and resid 195 and name C) (segid 3A4 and resid 195 and name O)	1.23	0.00	0.01
	assign (segid 3A4 and resid 195 and name C) (segid 3A4 and resid 196 and name C)	3.03	0.01	0.02
	assign (segid 3A4 and resid 195 and name C) (segid 3A4 and resid 196 and name CA)	2.44	0.02	0.02
20	assign (segid 3A4 and resid 195 and name C) (segid 3A4 and resid 196 and name CB)	3.71	0.03	0.03
	assign (segid 3A4 and resid 195 and name C) (segid 3A4 and resid 196 and name N)	1.33	0.01	0.01
	assign (segid 3A4 and resid 195 and name C) (segid 3A4 and resid 196 and name O)	3.80	0.12	0.13
	assign (segid 3A4 and resid 195 and name C) (segid 3A4 and resid 197 and name C)	4.59	0.12	0.11
25	assign (segid 3A4 and resid 195 and name C) (segid 3A4 and resid 197 and name CA)	4.52	0.14	0.14
	assign (segid 3A4 and resid 195 and name C) (segid 3A4 and resid 197 and name CB)	5.21	0.18	0.18
	assign (segid 3A4 and resid 195 and name C) (segid 3A4 and resid 197 and name CG)	6.51	0.19	0.20
	assign (segid 3A4 and resid 195 and name C) (segid 3A4 and resid 197 and name N)	3.36	0.14	0.14
	assign (segid 3A4 and resid 195 and name C) (segid 3A4 and resid 197 and name O)	5.64	0.11	0.10
	assign (segid 3A4 and resid 195 and name C) (segid 3A4 and resid 198 and name C)	4.94	0.04	0.04
30	assign (segid 3A4 and resid 195 and name C) (segid 3A4 and resid 198 and name CA)	4.65	0.07	0.07
	assign (segid 3A4 and resid 195 and name C) (segid 3A4 and resid 198 and name CB)	4.52	0.13	0.13
	assign (segid 3A4 and resid 195 and name C) (segid 3A4 and resid 198 and name CG)	5.18	0.18	0.18
	assign (segid 3A4 and resid 195 and name C) (segid 3A4 and resid 198 and name N)	3.90	0.08	0.09
	assign (segid 3A4 and resid 195 and name C) (segid 3A4 and resid 198 and name O)	6.14	0.04	0.05
35	assign (segid 3A4 and resid 195 and name C) (segid 3A4 and resid 199 and name C)	6.14	0.14	0.15
	assign (segid 3A4 and resid 195 and name C) (segid 3A4 and resid 199 and name CA)	4.97	0.12	0.13
	assign (segid 3A4 and resid 195 and name C) (segid 3A4 and resid 199 and name CB)	4.47	0.20	0.20
	assign (segid 3A4 and resid 195 and name C) (segid 3A4 and resid 199 and name N)	4.14	0.07	0.07
	assign (segid 3A4 and resid 195 and name C) (segid 3A4 and resid 199 and name O)	7.27	0.14	0.13
40	assign (segid 3A4 and resid 195 and name C) (segid 3A4 and resid 200 and name CA)	7.46	0.23	0.23
	assign (segid 3A4 and resid 195 and name C) (segid 3A4 and resid 200 and name N)	6.15	0.21	0.20
	assign (segid 3A4 and resid 195 and name C) (segid 3A4 and resid 245 and name CB)	6.47	0.62	0.63
	assign (segid 3A4 and resid 195 and name CA) (segid 3A4 and resid 195 and name C)	1.51	0.01	0.01
	assign (segid 3A4 and resid 195 and name CA) (segid 3A4 and resid 195 and name CB)	1.52	0.01	0.02
45	assign (segid 3A4 and resid 195 and name CA) (segid 3A4 and resid 195 and name O)	2.38	0.02	0.01
	assign (segid 3A4 and resid 195 and name CA) (segid 3A4 and resid 196 and name C)	4.40	0.01	0.02
	assign (segid 3A4 and resid 195 and name CA) (segid 3A4 and resid 196 and name CA)	3.81	0.03	0.02
	assign (segid 3A4 and resid 195 and name CA) (segid 3A4 and resid 196 and name CB)	4.86	0.04	0.05
	assign (segid 3A4 and resid 195 and name CA) (segid 3A4 and resid 196 and name N)	2.44	0.03	0.02
50	assign (segid 3A4 and resid 195 and name CA) (segid 3A4 and resid 196 and name O)	5.25	0.14	0.13
	assign (segid 3A4 and resid 195 and name CA) (segid 3A4 and resid 197 and name C)	5.52	0.15	0.15
	assign (segid 3A4 and resid 195 and name CA) (segid 3A4 and resid 197 and name CA)	5.48	0.18	0.17
	assign (segid 3A4 and resid 195 and name CA) (segid 3A4 and resid 197 and name CB)	5.82	0.24	0.25
	assign (segid 3A4 and resid 195 and name CA) (segid 3A4 and resid 197 and name CG)	7.08	0.28	0.27
55	assign (segid 3A4 and resid 195 and name CA) (segid 3A4 and resid 197 and name N)	4.44	0.15	0.15
	assign (segid 3A4 and resid 195 and name CA) (segid 3A4 and resid 197 and name O)	6.64	0.13	0.14
	assign (segid 3A4 and resid 195 and name CA) (segid 3A4 and resid 198 and name C)	5.74	0.09	0.09
	assign (segid 3A4 and resid 195 and name CA) (segid 3A4 and resid 198 and name CA)	5.22	0.10	0.11
	assign (segid 3A4 and resid 195 and name CA) (segid 3A4 and resid 198 and name CB)	4.66	0.13	0.14
60	assign (segid 3A4 and resid 195 and name CA) (segid 3A4 and resid 198 and name CG)	5.01	0.19	0.19
	assign (segid 3A4 and resid 195 and name CA) (segid 3A4 and resid 198 and name N)	4.62	0.12	0.13
	assign (segid 3A4 and resid 195 and name CA) (segid 3A4 and resid 198 and name O)	6.94	0.10	0.10
	assign (segid 3A4 and resid 195 and name CA) (segid 3A4 and resid 199 and name C)	7.34	0.14	0.15
	assign (segid 3A4 and resid 195 and name CA) (segid 3A4 and resid 199 and name CA)	6.06	0.16	0.16
65	assign (segid 3A4 and resid 195 and name CA) (segid 3A4 and resid 199 and name CB)	5.66	0.24	0.23
	assign (segid 3A4 and resid 195 and name CA) (segid 3A4 and resid 199 and name N)	5.13	0.11	0.12
	assign (segid 3A4 and resid 195 and name CA) (segid 3A4 and resid 200 and name CA)	8.79	0.19	0.18
	assign (segid 3A4 and resid 195 and name CA) (segid 3A4 and resid 200 and name N)	7.44	0.16	0.17
	assign (segid 3A4 and resid 195 and name CA) (segid 3A4 and resid 201 and name CA)	10.04	0.15	0.14
70	assign (segid 3A4 and resid 195 and name CA) (segid 3A4 and resid 201 and name CB)	9.62	0.27	0.28
	assign (segid 3A4 and resid 195 and name CA) (segid 3A4 and resid 202 and name CA)	10.48	0.15	0.15
	assign (segid 3A4 and resid 195 and name CA) (segid 3A4 and resid 202 and name CB)	9.62	0.21	0.21
	assign (segid 3A4 and resid 195 and name CA) (segid 3A4 and resid 203 and name CA)	12.31	0.15	0.16
	assign (segid 3A4 and resid 195 and name CA) (segid 3A4 and resid 203 and name CB)	11.97	0.25	0.24
75	assign (segid 3A4 and resid 195 and name CA) (segid 3A4 and resid 204 and name CA)	14.38	0.14	0.14
	assign (segid 3A4 and resid 195 and name CA) (segid 3A4 and resid 204 and name CB)	14.10	0.21	0.21
	assign (segid 3A4 and resid 195 and name CA) (segid 3A4 and resid 205 and name CA)	15.22	0.11	0.10
	assign (segid 3A4 and resid 195 and name CA) (segid 3A4 and resid 205 and name CB)	14.45	0.14	0.13
	assign (segid 3A4 and resid 195 and name CA) (segid 3A4 and resid 206 and name CA)	16.50	0.19	0.19
80	assign (segid 3A4 and resid 195 and name CA) (segid 3A4 and resid 206 and name CB)	15.88	0.21	0.21
	assign (segid 3A4 and resid 195 and name CA) (segid 3A4 and resid 207 and name CA)	18.77	0.28	0.27
	assign (segid 3A4 and resid 195 and name CA) (segid 3A4 and resid 207 and name CB)	18.48	0.40	0.41

	assign (segid 3A4 and resid 195 and name CA)	(segid 3A4 and resid 219 and name CA)	18.45	0.62	0.63
	assign (segid 3A4 and resid 195 and name CA)	(segid 3A4 and resid 219 and name CB)	17.52	0.56	0.57
	assign (segid 3A4 and resid 195 and name CA)	(segid 3A4 and resid 220 and name CA)	16.60	0.86	0.85
	assign (segid 3A4 and resid 195 and name CA)	(segid 3A4 and resid 220 and name CB)	16.06	0.97	0.97
5	assign (segid 3A4 and resid 195 and name CA)	(segid 3A4 and resid 221 and name CA)	13.98	0.77	0.76
	assign (segid 3A4 and resid 195 and name CA)	(segid 3A4 and resid 221 and name CB)	13.06	0.71	0.71
	assign (segid 3A4 and resid 195 and name CA)	(segid 3A4 and resid 222 and name CA)	16.96	0.78	0.78
	assign (segid 3A4 and resid 195 and name CA)	(segid 3A4 and resid 222 and name CB)	18.06	0.76	0.76
	assign (segid 3A4 and resid 195 and name CA)	(segid 3A4 and resid 224 and name CA)	16.21	0.93	0.94
10	assign (segid 3A4 and resid 195 and name CA)	(segid 3A4 and resid 224 and name CB)	14.92	0.87	0.88
	assign (segid 3A4 and resid 195 and name CA)	(segid 3A4 and resid 225 and name CA)	15.88	1.26	1.26
	assign (segid 3A4 and resid 195 and name CA)	(segid 3A4 and resid 225 and name CB)	15.57	1.26	1.27
	assign (segid 3A4 and resid 195 and name CA)	(segid 3A4 and resid 240 and name CA)	14.45	0.98	0.97
	assign (segid 3A4 and resid 195 and name CA)	(segid 3A4 and resid 240 and name CB)	14.54	0.88	0.88
	assign (segid 3A4 and resid 195 and name CA)	(segid 3A4 and resid 241 and name CA)	11.29	1.16	1.16
15	assign (segid 3A4 and resid 195 and name CA)	(segid 3A4 and resid 241 and name CB)	11.20	1.37	1.36
	assign (segid 3A4 and resid 195 and name CA)	(segid 3A4 and resid 242 and name CA)	9.62	0.71	0.71
	assign (segid 3A4 and resid 195 and name CA)	(segid 3A4 and resid 242 and name CB)	10.29	0.67	0.68
	assign (segid 3A4 and resid 195 and name CA)	(segid 3A4 and resid 243 and name CA)	11.50	0.56	0.56
20	assign (segid 3A4 and resid 195 and name CA)	(segid 3A4 and resid 243 and name CB)	13.01	0.58	0.57
	assign (segid 3A4 and resid 195 and name CA)	(segid 3A4 and resid 244 and name CA)	10.79	0.71	0.70
	assign (segid 3A4 and resid 195 and name CA)	(segid 3A4 and resid 244 and name CB)	11.11	0.90	0.90
	assign (segid 3A4 and resid 195 and name CA)	(segid 3A4 and resid 245 and name CA)	7.08	0.65	0.65
	assign (segid 3A4 and resid 195 and name CA)	(segid 3A4 and resid 245 and name CB)	6.18	0.80	0.81
25	assign (segid 3A4 and resid 195 and name CA)	(segid 3A4 and resid 245 and name O)	6.80	0.38	0.38
	assign (segid 3A4 and resid 195 and name CA)	(segid 3A4 and resid 246 and name CA)	8.33	0.27	0.26
	assign (segid 3A4 and resid 195 and name CA)	(segid 3A4 and resid 246 and name CB)	9.23	0.21	0.22
	assign (segid 3A4 and resid 195 and name CA)	(segid 3A4 and resid 247 and name CA)	11.01	0.33	0.32
	assign (segid 3A4 and resid 195 and name CA)	(segid 3A4 and resid 247 and name CB)	12.03	0.40	0.39
30	assign (segid 3A4 and resid 195 and name CA)	(segid 3A4 and resid 248 and name CA)	9.46	0.39	0.38
	assign (segid 3A4 and resid 195 and name CA)	(segid 3A4 and resid 248 and name CB)	8.79	0.44	0.43
	assign (segid 3A4 and resid 195 and name CA)	(segid 3A4 and resid 249 and name CA)	7.71	0.69	0.69
	assign (segid 3A4 and resid 195 and name CA)	(segid 3A4 and resid 250 and name CA)	11.12	0.70	0.70
	assign (segid 3A4 and resid 195 and name CA)	(segid 3A4 and resid 250 and name CB)	11.87	0.58	0.58
35	assign (segid 3A4 and resid 195 and name CA)	(segid 3A4 and resid 251 and name CA)	13.00	0.69	0.69
	assign (segid 3A4 and resid 195 and name CA)	(segid 3A4 and resid 251 and name CB)	13.16	0.61	0.61
	assign (segid 3A4 and resid 195 and name CA)	(segid 3A4 and resid 252 and name CA)	11.68	0.93	0.92
	assign (segid 3A4 and resid 195 and name CA)	(segid 3A4 and resid 252 and name CB)	10.34	0.96	0.97
	assign (segid 3A4 and resid 195 and name CA)	(segid 3A4 and resid 253 and name CA)	12.30	1.02	1.03
40	assign (segid 3A4 and resid 195 and name CA)	(segid 3A4 and resid 254 and name CA)	15.41	0.94	0.93
	assign (segid 3A4 and resid 195 and name CA)	(segid 3A4 and resid 255 and name CA)	16.77	0.93	0.92
	assign (segid 3A4 and resid 195 and name CA)	(segid 3A4 and resid 256 and name CA)	16.70	1.06	1.06
	assign (segid 3A4 and resid 195 and name CB)	(segid 3A4 and resid 196 and name C)	5.45	0.07	0.07
	assign (segid 3A4 and resid 195 and name CB)	(segid 3A4 and resid 196 and name CA)	4.52	0.11	0.10
	assign (segid 3A4 and resid 195 and name CB)	(segid 3A4 and resid 196 and name CB)	5.40	0.13	0.13
45	assign (segid 3A4 and resid 195 and name CB)	(segid 3A4 and resid 196 and name N)	3.20	0.09	0.09
	assign (segid 3A4 and resid 195 and name CB)	(segid 3A4 and resid 196 and name O)	6.25	0.15	0.16
	assign (segid 3A4 and resid 195 and name CB)	(segid 3A4 and resid 197 and name C)	6.92	0.14	0.15
	assign (segid 3A4 and resid 195 and name CB)	(segid 3A4 and resid 197 and name CA)	6.85	0.13	0.13
	assign (segid 3A4 and resid 195 and name CB)	(segid 3A4 and resid 197 and name CB)	7.25	0.20	0.21
50	assign (segid 3A4 and resid 195 and name CB)	(segid 3A4 and resid 197 and name N)	5.69	0.11	0.10
	assign (segid 3A4 and resid 195 and name CB)	(segid 3A4 and resid 198 and name C)	6.87	0.15	0.16
	assign (segid 3A4 and resid 195 and name CB)	(segid 3A4 and resid 198 and name CA)	6.54	0.16	0.16
	assign (segid 3A4 and resid 195 and name CB)	(segid 3A4 and resid 198 and name CB)	5.90	0.20	0.19
	assign (segid 3A4 and resid 195 and name CB)	(segid 3A4 and resid 198 and name CG)	6.31	0.22	0.23
55	assign (segid 3A4 and resid 195 and name CB)	(segid 3A4 and resid 198 and name N)	6.04	0.14	0.15
	assign (segid 3A4 and resid 195 and name CB)	(segid 3A4 and resid 199 and name CA)	6.79	0.22	0.22
	assign (segid 3A4 and resid 195 and name CB)	(segid 3A4 and resid 199 and name CB)	6.13	0.28	0.28
	assign (segid 3A4 and resid 195 and name CB)	(segid 3A4 and resid 199 and name N)	6.11	0.18	0.17
60	assign (segid 3A4 and resid 195 and name CB)	(segid 3A4 and resid 200 and name CA)	9.74	0.21	0.21
	assign (segid 3A4 and resid 195 and name CB)	(segid 3A4 and resid 201 and name CA)	11.22	0.14	0.13
	assign (segid 3A4 and resid 195 and name CB)	(segid 3A4 and resid 201 and name CB)	10.89	0.26	0.26
	assign (segid 3A4 and resid 195 and name CB)	(segid 3A4 and resid 202 and name CA)	11.31	0.25	0.26
	assign (segid 3A4 and resid 195 and name CB)	(segid 3A4 and resid 202 and name CB)	10.33	0.34	0.33
65	assign (segid 3A4 and resid 195 and name CB)	(segid 3A4 and resid 203 and name CA)	12.99	0.27	0.27
	assign (segid 3A4 and resid 195 and name CB)	(segid 3A4 and resid 203 and name CB)	12.59	0.33	0.33
	assign (segid 3A4 and resid 195 and name CB)	(segid 3A4 and resid 204 and name CA)	15.32	0.22	0.22
	assign (segid 3A4 and resid 195 and name CB)	(segid 3A4 and resid 204 and name CB)	15.14	0.26	0.27
	assign (segid 3A4 and resid 195 and name CB)	(segid 3A4 and resid 205 and name CA)	16.17	0.20	0.20
70	assign (segid 3A4 and resid 195 and name CB)	(segid 3A4 and resid 205 and name CB)	15.42	0.17	0.18
	assign (segid 3A4 and resid 195 and name CB)	(segid 3A4 and resid 206 and name CA)	17.18	0.32	0.32
	assign (segid 3A4 and resid 195 and name CB)	(segid 3A4 and resid 206 and name CB)	16.45	0.35	0.35
	assign (segid 3A4 and resid 195 and name CB)	(segid 3A4 and resid 207 and name CA)	19.50	0.38	0.39
	assign (segid 3A4 and resid 195 and name CB)	(segid 3A4 and resid 207 and name CB)	19.24	0.50	0.50
75	assign (segid 3A4 and resid 195 and name CB)	(segid 3A4 and resid 219 and name CB)	18.72	0.59	0.59
	assign (segid 3A4 and resid 195 and name CB)	(segid 3A4 and resid 220 and name CA)	17.57	0.94	0.93
	assign (segid 3A4 and resid 195 and name CB)	(segid 3A4 and resid 220 and name CB)	17.03	1.03	1.02
	assign (segid 3A4 and resid 195 and name CB)	(segid 3A4 and resid 221 and name CA)	14.93	0.85	0.85
	assign (segid 3A4 and resid 195 and name CB)	(segid 3A4 and resid 221 and name CB)	14.10	0.78	0.78
80	assign (segid 3A4 and resid 195 and name CB)	(segid 3A4 and resid 222 and name CA)	17.88	0.88	0.87
	assign (segid 3A4 and resid 195 and name CB)	(segid 3A4 and resid 224 and name CA)	16.77	1.09	1.09
	assign (segid 3A4 and resid 195 and name CB)	(segid 3A4 and resid 224 and name CB)	15.48	1.02	1.03
	assign (segid 3A4 and resid 195 and name CB)	(segid 3A4 and resid 225 and name CA)	16.42	1.40	1.40

	assign (segid 3A4 and resid 195 and name CB)	(segid 3A4 and resid 225 and name CB)	16.21	1.38	1.38
	assign (segid 3A4 and resid 195 and name CB)	(segid 3A4 and resid 240 and name CA)	14.15	1.15	1.14
	assign (segid 3A4 and resid 195 and name CB)	(segid 3A4 and resid 240 and name CB)	14.09	1.05	1.05
	assign (segid 3A4 and resid 195 and name CB)	(segid 3A4 and resid 241 and name CA)	11.14	1.34	1.33
	assign (segid 3A4 and resid 195 and name CB)	(segid 3A4 and resid 241 and name CB)	11.02	1.55	1.55
5	assign (segid 3A4 and resid 195 and name CB)	(segid 3A4 and resid 242 and name CA)	9.11	0.86	0.86
	assign (segid 3A4 and resid 195 and name CB)	(segid 3A4 and resid 242 and name CB)	9.59	0.78	0.78
	assign (segid 3A4 and resid 195 and name CB)	(segid 3A4 and resid 243 and name CA)	11.19	0.68	0.68
	assign (segid 3A4 and resid 195 and name CB)	(segid 3A4 and resid 243 and name CB)	12.69	0.69	0.69
	assign (segid 3A4 and resid 195 and name CB)	(segid 3A4 and resid 244 and name CA)	10.96	0.84	0.85
10	assign (segid 3A4 and resid 195 and name CB)	(segid 3A4 and resid 244 and name CB)	11.36	1.01	1.01
	assign (segid 3A4 and resid 195 and name CB)	(segid 3A4 and resid 245 and name CA)	7.33	0.78	0.77
	assign (segid 3A4 and resid 195 and name CB)	(segid 3A4 and resid 245 and name CB)	6.26	0.90	0.90
	assign (segid 3A4 and resid 195 and name CB)	(segid 3A4 and resid 246 and name CA)	8.21	0.42	0.41
	assign (segid 3A4 and resid 195 and name CB)	(segid 3A4 and resid 246 and name CB)	8.90	0.37	0.36
	assign (segid 3A4 and resid 195 and name CB)	(segid 3A4 and resid 247 and name CA)	11.25	0.48	0.48
15	assign (segid 3A4 and resid 195 and name CB)	(segid 3A4 and resid 247 and name CB)	12.29	0.52	0.52
	assign (segid 3A4 and resid 195 and name CB)	(segid 3A4 and resid 248 and name CA)	10.19	0.52	0.52
	assign (segid 3A4 and resid 195 and name CB)	(segid 3A4 and resid 248 and name CB)	9.62	0.52	0.52
	assign (segid 3A4 and resid 195 and name CB)	(segid 3A4 and resid 249 and name CA)	8.29	0.77	0.78
20	assign (segid 3A4 and resid 195 and name CB)	(segid 3A4 and resid 250 and name CA)	11.46	0.76	0.76
	assign (segid 3A4 and resid 195 and name CB)	(segid 3A4 and resid 250 and name CB)	12.08	0.64	0.64
	assign (segid 3A4 and resid 195 and name CB)	(segid 3A4 and resid 251 and name CA)	13.69	0.76	0.76
	assign (segid 3A4 and resid 195 and name CB)	(segid 3A4 and resid 251 and name CB)	13.91	0.69	0.70
	assign (segid 3A4 and resid 195 and name CB)	(segid 3A4 and resid 252 and name CA)	12.60	0.97	0.96
25	assign (segid 3A4 and resid 195 and name CB)	(segid 3A4 and resid 252 and name CB)	11.34	1.01	1.00
	assign (segid 3A4 and resid 195 and name CB)	(segid 3A4 and resid 253 and name CA)	12.92	1.06	1.06
	assign (segid 3A4 and resid 195 and name CB)	(segid 3A4 and resid 254 and name CA)	15.91	1.00	0.99
	assign (segid 3A4 and resid 195 and name CB)	(segid 3A4 and resid 255 and name CA)	17.54	0.92	0.92
	assign (segid 3A4 and resid 195 and name CB)	(segid 3A4 and resid 256 and name CA)	17.59	1.10	1.10
30	assign (segid 3A4 and resid 195 and name CB)	(segid 3A4 and resid 195 and name C)	2.47	0.02	0.02
	assign (segid 3A4 and resid 195 and name N)	(segid 3A4 and resid 195 and name CA)	1.46	0.00	0.00
	assign (segid 3A4 and resid 195 and name N)	(segid 3A4 and resid 195 and name CB)	2.46	0.03	0.03
	assign (segid 3A4 and resid 195 and name N)	(segid 3A4 and resid 195 and name O)	3.50	0.03	0.03
	assign (segid 3A4 and resid 195 and name N)	(segid 3A4 and resid 196 and name C)	4.71	0.03	0.04
35	assign (segid 3A4 and resid 195 and name N)	(segid 3A4 and resid 196 and name CA)	4.23	0.03	0.04
	assign (segid 3A4 and resid 195 and name N)	(segid 3A4 and resid 196 and name CB)	4.99	0.04	0.04
	assign (segid 3A4 and resid 195 and name N)	(segid 3A4 and resid 196 and name N)	2.83	0.04	0.04
	assign (segid 3A4 and resid 195 and name N)	(segid 3A4 and resid 196 and name O)	5.74	0.12	0.11
	assign (segid 3A4 and resid 195 and name N)	(segid 3A4 and resid 197 and name C)	5.66	0.11	0.12
40	assign (segid 3A4 and resid 195 and name N)	(segid 3A4 and resid 197 and name CA)	5.35	0.16	0.17
	assign (segid 3A4 and resid 195 and name N)	(segid 3A4 and resid 197 and name CB)	5.33	0.26	0.26
	assign (segid 3A4 and resid 195 and name N)	(segid 3A4 and resid 197 and name CG)	6.60	0.30	0.30
	assign (segid 3A4 and resid 195 and name N)	(segid 3A4 and resid 197 and name N)	4.38	0.14	0.13
	assign (segid 3A4 and resid 195 and name N)	(segid 3A4 and resid 197 and name O)	6.87	0.10	0.10
45	assign (segid 3A4 and resid 195 and name N)	(segid 3A4 and resid 198 and name C)	6.50	0.04	0.04
	assign (segid 3A4 and resid 195 and name N)	(segid 3A4 and resid 198 and name CA)	5.69	0.07	0.07
	assign (segid 3A4 and resid 195 and name N)	(segid 3A4 and resid 198 and name CB)	5.16	0.10	0.10
	assign (segid 3A4 and resid 195 and name N)	(segid 3A4 and resid 198 and name CG)	5.11	0.19	0.20
	assign (segid 3A4 and resid 195 and name N)	(segid 3A4 and resid 198 and name N)	4.88	0.08	0.07
50	assign (segid 3A4 and resid 195 and name N)	(segid 3A4 and resid 198 and name O)	7.71	0.05	0.06
	assign (segid 3A4 and resid 195 and name N)	(segid 3A4 and resid 199 and name CA)	7.15	0.12	0.12
	assign (segid 3A4 and resid 195 and name N)	(segid 3A4 and resid 199 and name CB)	6.85	0.19	0.20
	assign (segid 3A4 and resid 195 and name N)	(segid 3A4 and resid 199 and name N)	6.07	0.08	0.07
	assign (segid 3A4 and resid 195 and name N)	(segid 3A4 and resid 199 and name CB)	3.27	0.04	0.03
55	assign (segid 3A4 and resid 195 and name O)	(segid 3A4 and resid 196 and name C)	3.00	0.04	0.04
	assign (segid 3A4 and resid 195 and name O)	(segid 3A4 and resid 196 and name CA)	2.78	0.04	0.03
	assign (segid 3A4 and resid 195 and name O)	(segid 3A4 and resid 196 and name CB)	4.25	0.04	0.04
	assign (segid 3A4 and resid 195 and name O)	(segid 3A4 and resid 196 and name N)	2.25	0.02	0.01
	assign (segid 3A4 and resid 195 and name O)	(segid 3A4 and resid 196 and name O)	3.39	0.14	0.15
60	assign (segid 3A4 and resid 195 and name O)	(segid 3A4 and resid 197 and name C)	4.17	0.20	0.20
	assign (segid 3A4 and resid 195 and name O)	(segid 3A4 and resid 197 and name CA)	4.47	0.20	0.20
	assign (segid 3A4 and resid 195 and name O)	(segid 3A4 and resid 197 and name CB)	5.38	0.20	0.20
	assign (segid 3A4 and resid 195 and name O)	(segid 3A4 and resid 197 and name CG)	6.53	0.23	0.24
	assign (segid 3A4 and resid 195 and name O)	(segid 3A4 and resid 197 and name N)	3.53	0.18	0.18
65	assign (segid 3A4 and resid 195 and name O)	(segid 3A4 and resid 197 and name O)	5.06	0.19	0.18
	assign (segid 3A4 and resid 195 and name O)	(segid 3A4 and resid 198 and name C)	3.91	0.11	0.10
	assign (segid 3A4 and resid 195 and name O)	(segid 3A4 and resid 198 and name CA)	3.90	0.13	0.12
	assign (segid 3A4 and resid 195 and name O)	(segid 3A4 and resid 198 and name CB)	3.87	0.12	0.12
	assign (segid 3A4 and resid 195 and name O)	(segid 3A4 and resid 198 and name CG)	4.84	0.15	0.15
70	assign (segid 3A4 and resid 195 and name O)	(segid 3A4 and resid 198 and name N)	3.42	0.18	0.17
	assign (segid 3A4 and resid 195 and name O)	(segid 3A4 and resid 198 and name O)	5.08	0.10	0.10
	assign (segid 3A4 and resid 195 and name O)	(segid 3A4 and resid 199 and name C)	5.03	0.15	0.15
	assign (segid 3A4 and resid 195 and name O)	(segid 3A4 and resid 199 and name CA)	3.78	0.13	0.14
	assign (segid 3A4 and resid 195 and name O)	(segid 3A4 and resid 199 and name CB)	3.38	0.19	0.19
75	assign (segid 3A4 and resid 195 and name O)	(segid 3A4 and resid 199 and name N)	3.00	0.11	0.11
	assign (segid 3A4 and resid 195 and name O)	(segid 3A4 and resid 199 and name O)	6.11	0.14	0.14
	assign (segid 3A4 and resid 195 and name O)	(segid 3A4 and resid 200 and name C)	7.39	0.18	0.17
	assign (segid 3A4 and resid 195 and name O)	(segid 3A4 and resid 200 and name CA)	6.54	0.20	0.20
	assign (segid 3A4 and resid 195 and name O)	(segid 3A4 and resid 200 and name N)	5.16	0.19	0.19
80	assign (segid 3A4 and resid 195 and name O)	(segid 3A4 and resid 201 and name N)	7.05	0.12	0.12
	assign (segid 3A4 and resid 195 and name O)	(segid 3A4 and resid 202 and name CB)	7.74	0.17	0.16
	assign (segid 3A4 and resid 195 and name O)	(segid 3A4 and resid 202 and name N)	7.78	0.06	0.05

	assign (segid 3A4 and resid 195 and name O) (segid 3A4 and resid 245 and name C)	7.24	0.32	0.31
	assign (segid 3A4 and resid 195 and name O) (segid 3A4 and resid 245 and name CA)	6.73	0.44	0.44
	assign (segid 3A4 and resid 195 and name O) (segid 3A4 and resid 245 and name CB)	5.76	0.52	0.52
	assign (segid 3A4 and resid 195 and name O) (segid 3A4 and resid 245 and name O)	7.11	0.36	0.35
5	assign (segid 3A4 and resid 196 and name C) (segid 3A4 and resid 196 and name CB)	2.48	0.03	0.04
	assign (segid 3A4 and resid 196 and name C) (segid 3A4 and resid 196 and name O)	1.23	0.00	0.01
	assign (segid 3A4 and resid 196 and name C) (segid 3A4 and resid 197 and name C)	2.98	0.07	0.08
	assign (segid 3A4 and resid 196 and name C) (segid 3A4 and resid 197 and name CA)	2.44	0.02	0.02
	assign (segid 3A4 and resid 196 and name C) (segid 3A4 and resid 197 and name CB)	3.70	0.02	0.02
10	assign (segid 3A4 and resid 196 and name C) (segid 3A4 and resid 197 and name CG)	4.95	0.02	0.03
	assign (segid 3A4 and resid 196 and name C) (segid 3A4 and resid 197 and name N)	1.33	0.01	0.01
	assign (segid 3A4 and resid 196 and name C) (segid 3A4 and resid 197 and name O)	3.79	0.08	0.08
	assign (segid 3A4 and resid 196 and name C) (segid 3A4 and resid 198 and name C)	4.61	0.21	0.21
	assign (segid 3A4 and resid 196 and name C) (segid 3A4 and resid 198 and name CA)	4.48	0.18	0.18
	assign (segid 3A4 and resid 196 and name C) (segid 3A4 and resid 198 and name CB)	5.28	0.22	0.22
15	assign (segid 3A4 and resid 196 and name C) (segid 3A4 and resid 198 and name CG)	6.01	0.23	0.24
	assign (segid 3A4 and resid 196 and name C) (segid 3A4 and resid 198 and name N)	3.29	0.14	0.15
	assign (segid 3A4 and resid 196 and name C) (segid 3A4 and resid 198 and name O)	5.67	0.24	0.24
	assign (segid 3A4 and resid 196 and name C) (segid 3A4 and resid 199 and name C)	5.13	0.32	0.32
	assign (segid 3A4 and resid 196 and name C) (segid 3A4 and resid 199 and name CA)	4.65	0.22	0.23
20	assign (segid 3A4 and resid 196 and name C) (segid 3A4 and resid 199 and name CB)	4.37	0.24	0.24
	assign (segid 3A4 and resid 196 and name C) (segid 3A4 and resid 199 and name N)	3.93	0.22	0.22
	assign (segid 3A4 and resid 196 and name C) (segid 3A4 and resid 199 and name O)	6.34	0.34	0.34
	assign (segid 3A4 and resid 196 and name C) (segid 3A4 and resid 200 and name C)	6.54	0.40	0.40
	assign (segid 3A4 and resid 196 and name C) (segid 3A4 and resid 200 and name CA)	5.48	0.44	0.43
25	assign (segid 3A4 and resid 196 and name C) (segid 3A4 and resid 200 and name N)	4.51	0.39	0.40
	assign (segid 3A4 and resid 196 and name C) (segid 3A4 and resid 201 and name N)	6.37	0.35	0.35
	assign (segid 3A4 and resid 196 and name C) (segid 3A4 and resid 196 and name C)	1.52	0.01	0.01
	assign (segid 3A4 and resid 196 and name CA) (segid 3A4 and resid 196 and name CB)	1.52	0.02	0.01
	assign (segid 3A4 and resid 196 and name CA) (segid 3A4 and resid 196 and name O)	2.39	0.04	0.03
30	assign (segid 3A4 and resid 196 and name CA) (segid 3A4 and resid 197 and name C)	4.38	0.04	0.04
	assign (segid 3A4 and resid 196 and name CA) (segid 3A4 and resid 197 and name CA)	3.80	0.01	0.01
	assign (segid 3A4 and resid 196 and name CA) (segid 3A4 and resid 197 and name CB)	4.83	0.05	0.05
	assign (segid 3A4 and resid 196 and name CA) (segid 3A4 and resid 197 and name CG)	6.21	0.04	0.04
	assign (segid 3A4 and resid 196 and name CA) (segid 3A4 and resid 197 and name N)	2.43	0.03	0.02
35	assign (segid 3A4 and resid 196 and name CA) (segid 3A4 and resid 197 and name O)	5.25	0.07	0.07
	assign (segid 3A4 and resid 196 and name CA) (segid 3A4 and resid 198 and name C)	5.56	0.15	0.16
	assign (segid 3A4 and resid 196 and name CA) (segid 3A4 and resid 198 and name CA)	5.50	0.13	0.12
	assign (segid 3A4 and resid 196 and name CA) (segid 3A4 and resid 198 and name CB)	5.99	0.18	0.18
	assign (segid 3A4 and resid 196 and name CA) (segid 3A4 and resid 198 and name CG)	6.73	0.21	0.21
40	assign (segid 3A4 and resid 196 and name CA) (segid 3A4 and resid 198 and name N)	4.41	0.09	0.08
	assign (segid 3A4 and resid 196 and name CA) (segid 3A4 and resid 198 and name O)	6.67	0.18	0.18
	assign (segid 3A4 and resid 196 and name CA) (segid 3A4 and resid 199 and name C)	5.90	0.31	0.30
	assign (segid 3A4 and resid 196 and name CA) (segid 3A4 and resid 199 and name CA)	5.20	0.20	0.20
	assign (segid 3A4 and resid 196 and name CA) (segid 3A4 and resid 199 and name CB)	4.49	0.23	0.23
45	assign (segid 3A4 and resid 196 and name CA) (segid 3A4 and resid 199 and name N)	4.65	0.18	0.17
	assign (segid 3A4 and resid 196 and name CA) (segid 3A4 and resid 199 and name O)	7.06	0.32	0.33
	assign (segid 3A4 and resid 196 and name CA) (segid 3A4 and resid 200 and name CA)	6.54	0.42	0.43
	assign (segid 3A4 and resid 196 and name CA) (segid 3A4 and resid 200 and name N)	5.50	0.37	0.37
	assign (segid 3A4 and resid 196 and name CA) (segid 3A4 and resid 201 and name CA)	8.92	0.28	0.27
50	assign (segid 3A4 and resid 196 and name CA) (segid 3A4 and resid 201 and name CB)	8.93	0.27	0.27
	assign (segid 3A4 and resid 196 and name CA) (segid 3A4 and resid 202 and name CA)	10.09	0.29	0.28
	assign (segid 3A4 and resid 196 and name CA) (segid 3A4 and resid 202 and name CB)	9.58	0.31	0.30
	assign (segid 3A4 and resid 196 and name CA) (segid 3A4 and resid 203 and name CA)	10.91	0.36	0.35
	assign (segid 3A4 and resid 196 and name CA) (segid 3A4 and resid 203 and name CB)	10.19	0.43	0.42
55	assign (segid 3A4 and resid 196 and name CA) (segid 3A4 and resid 204 and name CA)	12.70	0.38	0.37
	assign (segid 3A4 and resid 196 and name CA) (segid 3A4 and resid 204 and name CB)	12.31	0.30	0.30
	assign (segid 3A4 and resid 196 and name CA) (segid 3A4 and resid 205 and name CA)	14.42	0.36	0.36
	assign (segid 3A4 and resid 196 and name CA) (segid 3A4 and resid 205 and name CB)	13.98	0.41	0.40
	assign (segid 3A4 and resid 196 and name CA) (segid 3A4 and resid 206 and name CA)	15.73	0.30	0.30
60	assign (segid 3A4 and resid 196 and name CA) (segid 3A4 and resid 206 and name CB)	15.10	0.31	0.31
	assign (segid 3A4 and resid 196 and name CA) (segid 3A4 and resid 207 and name CA)	17.33	0.39	0.39
	assign (segid 3A4 and resid 196 and name CA) (segid 3A4 and resid 207 and name CB)	16.78	0.50	0.49
	assign (segid 3A4 and resid 196 and name CA) (segid 3A4 and resid 209 and name CB)	18.10	0.46	0.46
	assign (segid 3A4 and resid 196 and name CA) (segid 3A4 and resid 220 and name CA)	17.98	0.76	0.75
65	assign (segid 3A4 and resid 196 and name CA) (segid 3A4 and resid 220 and name CB)	17.68	0.91	0.91
	assign (segid 3A4 and resid 196 and name CA) (segid 3A4 and resid 221 and name CA)	14.96	0.66	0.66
	assign (segid 3A4 and resid 196 and name CA) (segid 3A4 and resid 221 and name CB)	13.81	0.61	0.60
	assign (segid 3A4 and resid 196 and name CA) (segid 3A4 and resid 222 and name CA)	17.44	0.65	0.64
	assign (segid 3A4 and resid 196 and name CA) (segid 3A4 and resid 222 and name CB)	18.37	0.63	0.64
70	assign (segid 3A4 and resid 196 and name CA) (segid 3A4 and resid 224 and name CA)	17.66	0.79	0.79
	assign (segid 3A4 and resid 196 and name CA) (segid 3A4 and resid 224 and name CB)	16.53	0.76	0.75
	assign (segid 3A4 and resid 196 and name CA) (segid 3A4 and resid 225 and name CA)	16.61	1.10	1.11
	assign (segid 3A4 and resid 196 and name CA) (segid 3A4 and resid 225 and name CB)	16.01	1.09	1.08
	assign (segid 3A4 and resid 196 and name CA) (segid 3A4 and resid 240 and name CA)	15.87	0.92	0.92
75	assign (segid 3A4 and resid 196 and name CA) (segid 3A4 and resid 240 and name CB)	16.07	0.84	0.84
	assign (segid 3A4 and resid 196 and name CA) (segid 3A4 and resid 241 and name CA)	12.34	0.99	0.99
	assign (segid 3A4 and resid 196 and name CA) (segid 3A4 and resid 241 and name CB)	11.84	1.19	1.19
	assign (segid 3A4 and resid 196 and name CA) (segid 3A4 and resid 242 and name CA)	11.52	0.63	0.63
	assign (segid 3A4 and resid 196 and name CA) (segid 3A4 and resid 242 and name CB)	12.19	0.70	0.71
80	assign (segid 3A4 and resid 196 and name CA) (segid 3A4 and resid 243 and name CA)	13.99	0.53	0.52
	assign (segid 3A4 and resid 196 and name CA) (segid 3A4 and resid 243 and name CB)	15.43	0.54	0.54
	assign (segid 3A4 and resid 196 and name CA) (segid 3A4 and resid 244 and name CA)	12.86	0.59	0.58

	assign (segid 3A4 and resid 196 and name CA)	(segid 3A4 and resid 244 and name CB)	12.77	0.79	0.79
	assign (segid 3A4 and resid 196 and name CA)	(segid 3A4 and resid 245 and name CA)	9.46	0.44	0.43
	assign (segid 3A4 and resid 196 and name CA)	(segid 3A4 and resid 245 and name CB)	8.44	0.52	0.52
	assign (segid 3A4 and resid 196 and name CA)	(segid 3A4 and resid 246 and name CA)	11.58	0.34	0.35
5	assign (segid 3A4 and resid 196 and name CA)	(segid 3A4 and resid 246 and name CB)	12.50	0.31	0.32
	assign (segid 3A4 and resid 196 and name CA)	(segid 3A4 and resid 247 and name CA)	14.04	0.28	0.28
	assign (segid 3A4 and resid 196 and name CA)	(segid 3A4 and resid 247 and name CB)	14.86	0.34	0.35
	assign (segid 3A4 and resid 196 and name CA)	(segid 3A4 and resid 248 and name CA)	12.04	0.28	0.28
	assign (segid 3A4 and resid 196 and name CA)	(segid 3A4 and resid 248 and name CB)	11.03	0.32	0.32
10	assign (segid 3A4 and resid 196 and name CA)	(segid 3A4 and resid 249 and name CA)	10.92	0.71	0.70
	assign (segid 3A4 and resid 196 and name CA)	(segid 3A4 and resid 250 and name CA)	14.53	0.71	0.71
	assign (segid 3A4 and resid 196 and name CA)	(segid 3A4 and resid 250 and name CB)	15.34	0.58	0.58
	assign (segid 3A4 and resid 196 and name CA)	(segid 3A4 and resid 251 and name CA)	15.91	0.65	0.66
	assign (segid 3A4 and resid 196 and name CA)	(segid 3A4 and resid 251 and name CB)	15.88	0.56	0.55
15	assign (segid 3A4 and resid 196 and name CA)	(segid 3A4 and resid 252 and name CA)	14.26	0.93	0.92
	assign (segid 3A4 and resid 196 and name CA)	(segid 3A4 and resid 252 and name CB)	12.81	0.96	0.96
	assign (segid 3A4 and resid 196 and name CA)	(segid 3A4 and resid 253 and name CA)	15.32	1.05	1.04
	assign (segid 3A4 and resid 196 and name CB)	(segid 3A4 and resid 197 and name C)	5.36	0.10	0.10
	assign (segid 3A4 and resid 196 and name CB)	(segid 3A4 and resid 197 and name CA)	4.43	0.08	0.08
20	assign (segid 3A4 and resid 196 and name CB)	(segid 3A4 and resid 197 and name CB)	5.29	0.07	0.06
	assign (segid 3A4 and resid 196 and name CB)	(segid 3A4 and resid 197 and name CG)	6.70	0.07	0.07
	assign (segid 3A4 and resid 196 and name CB)	(segid 3A4 and resid 197 and name N)	3.09	0.09	0.09
	assign (segid 3A4 and resid 196 and name CB)	(segid 3A4 and resid 197 and name O)	6.19	0.12	0.11
	assign (segid 3A4 and resid 196 and name CB)	(segid 3A4 and resid 198 and name C)	6.95	0.19	0.19
25	assign (segid 3A4 and resid 196 and name CB)	(segid 3A4 and resid 198 and name CA)	6.83	0.15	0.15
	assign (segid 3A4 and resid 196 and name CB)	(segid 3A4 and resid 198 and name CB)	7.39	0.18	0.18
	assign (segid 3A4 and resid 196 and name CB)	(segid 3A4 and resid 198 and name N)	5.62	0.13	0.13
	assign (segid 3A4 and resid 196 and name CB)	(segid 3A4 and resid 199 and name C)	7.08	0.36	0.36
	assign (segid 3A4 and resid 196 and name CB)	(segid 3A4 and resid 199 and name CA)	6.55	0.22	0.22
30	assign (segid 3A4 and resid 196 and name CB)	(segid 3A4 and resid 199 and name CB)	5.77	0.24	0.24
	assign (segid 3A4 and resid 196 and name CB)	(segid 3A4 and resid 199 and name N)	6.08	0.19	0.20
	assign (segid 3A4 and resid 196 and name CB)	(segid 3A4 and resid 200 and name CA)	7.38	0.53	0.53
	assign (segid 3A4 and resid 196 and name CB)	(segid 3A4 and resid 200 and name N)	6.53	0.44	0.45
	assign (segid 3A4 and resid 196 and name CB)	(segid 3A4 and resid 201 and name CA)	9.97	0.36	0.36
35	assign (segid 3A4 and resid 196 and name CB)	(segid 3A4 and resid 201 and name CB)	10.03	0.33	0.33
	assign (segid 3A4 and resid 196 and name CB)	(segid 3A4 and resid 202 and name CA)	11.39	0.34	0.34
	assign (segid 3A4 and resid 196 and name CB)	(segid 3A4 and resid 202 and name CB)	10.95	0.35	0.35
	assign (segid 3A4 and resid 196 and name CB)	(segid 3A4 and resid 203 and name CA)	11.94	0.45	0.45
	assign (segid 3A4 and resid 196 and name CB)	(segid 3A4 and resid 203 and name CB)	11.09	0.52	0.53
40	assign (segid 3A4 and resid 196 and name CB)	(segid 3A4 and resid 204 and name CA)	13.57	0.49	0.49
	assign (segid 3A4 and resid 196 and name CB)	(segid 3A4 and resid 204 and name CB)	13.12	0.42	0.41
	assign (segid 3A4 and resid 196 and name CB)	(segid 3A4 and resid 205 and name CA)	15.54	0.45	0.46
	assign (segid 3A4 and resid 196 and name CB)	(segid 3A4 and resid 205 and name CB)	15.18	0.48	0.47
	assign (segid 3A4 and resid 196 and name CB)	(segid 3A4 and resid 206 and name CA)	16.88	0.40	0.40
45	assign (segid 3A4 and resid 196 and name CB)	(segid 3A4 and resid 206 and name CB)	16.24	0.40	0.40
	assign (segid 3A4 and resid 196 and name CB)	(segid 3A4 and resid 207 and name CA)	18.27	0.50	0.49
	assign (segid 3A4 and resid 196 and name CB)	(segid 3A4 and resid 207 and name CB)	17.61	0.58	0.58
	assign (segid 3A4 and resid 196 and name CB)	(segid 3A4 and resid 219 and name CB)	19.30	0.44	0.45
	assign (segid 3A4 and resid 196 and name CB)	(segid 3A4 and resid 221 and name CA)	16.35	0.63	0.63
50	assign (segid 3A4 and resid 196 and name CB)	(segid 3A4 and resid 221 and name CB)	15.16	0.58	0.57
	assign (segid 3A4 and resid 196 and name CB)	(segid 3A4 and resid 222 and name CA)	18.79	0.62	0.62
	assign (segid 3A4 and resid 196 and name CB)	(segid 3A4 and resid 224 and name CB)	18.02	0.75	0.74
	assign (segid 3A4 and resid 196 and name CB)	(segid 3A4 and resid 225 and name CA)	18.04	1.09	1.10
	assign (segid 3A4 and resid 196 and name CB)	(segid 3A4 and resid 225 and name CB)	17.40	1.06	1.06
55	assign (segid 3A4 and resid 196 and name CB)	(segid 3A4 and resid 240 and name CA)	17.21	0.98	0.99
	assign (segid 3A4 and resid 196 and name CB)	(segid 3A4 and resid 240 and name CB)	17.37	0.91	0.90
	assign (segid 3A4 and resid 196 and name CB)	(segid 3A4 and resid 241 and name CA)	13.69	1.03	1.03
	assign (segid 3A4 and resid 196 and name CB)	(segid 3A4 and resid 241 and name CB)	13.12	1.24	1.24
	assign (segid 3A4 and resid 196 and name CB)	(segid 3A4 and resid 242 and name CA)	12.81	0.67	0.68
60	assign (segid 3A4 and resid 196 and name CB)	(segid 3A4 and resid 242 and name CB)	13.39	0.74	0.75
	assign (segid 3A4 and resid 196 and name CB)	(segid 3A4 and resid 243 and name CA)	15.38	0.55	0.54
	assign (segid 3A4 and resid 196 and name CB)	(segid 3A4 and resid 243 and name CB)	16.83	0.57	0.57
	assign (segid 3A4 and resid 196 and name CB)	(segid 3A4 and resid 244 and name CA)	14.35	0.59	0.59
	assign (segid 3A4 and resid 196 and name CB)	(segid 3A4 and resid 244 and name CB)	14.27	0.79	0.79
65	assign (segid 3A4 and resid 196 and name CB)	(segid 3A4 and resid 245 and name CA)	10.93	0.44	0.43
	assign (segid 3A4 and resid 196 and name CB)	(segid 3A4 and resid 245 and name CB)	9.88	0.54	0.54
	assign (segid 3A4 and resid 196 and name CB)	(segid 3A4 and resid 246 and name CA)	12.91	0.32	0.31
	assign (segid 3A4 and resid 196 and name CB)	(segid 3A4 and resid 246 and name CB)	13.79	0.29	0.29
	assign (segid 3A4 and resid 196 and name CB)	(segid 3A4 and resid 247 and name CA)	15.44	0.27	0.27
70	assign (segid 3A4 and resid 196 and name CB)	(segid 3A4 and resid 247 and name CB)	16.30	0.32	0.33
	assign (segid 3A4 and resid 196 and name CB)	(segid 3A4 and resid 248 and name CA)	13.41	0.26	0.27
	assign (segid 3A4 and resid 196 and name CB)	(segid 3A4 and resid 248 and name CB)	12.43	0.31	0.32
	assign (segid 3A4 and resid 196 and name CB)	(segid 3A4 and resid 249 and name CA)	12.09	0.68	0.69
	assign (segid 3A4 and resid 196 and name CB)	(segid 3A4 and resid 250 and name CA)	15.68	0.71	0.72
75	assign (segid 3A4 and resid 196 and name CB)	(segid 3A4 and resid 250 and name CB)	16.54	0.59	0.58
	assign (segid 3A4 and resid 196 and name CB)	(segid 3A4 and resid 251 and name CA)	17.11	0.68	0.67
	assign (segid 3A4 and resid 196 and name CB)	(segid 3A4 and resid 251 and name CB)	17.13	0.56	0.56
	assign (segid 3A4 and resid 196 and name CB)	(segid 3A4 and resid 252 and name CA)	15.25	0.95	0.95
	assign (segid 3A4 and resid 196 and name CB)	(segid 3A4 and resid 252 and name CB)	13.78	0.98	0.98
80	assign (segid 3A4 and resid 196 and name CB)	(segid 3A4 and resid 253 and name CA)	16.14	1.09	1.08
	assign (segid 3A4 and resid 196 and name N)	(segid 3A4 and resid 196 and name C)	2.44	0.01	0.02
	assign (segid 3A4 and resid 196 and name N)	(segid 3A4 and resid 196 and name CA)	1.46	0.01	0.01
	assign (segid 3A4 and resid 196 and name N)	(segid 3A4 and resid 196 and name CB)	2.45	0.02	0.02

	assign (segid 3A4 and resid 196 and name N)	(segid 3A4 and resid 196 and name O)	3.46	0.08	0.07
	assign (segid 3A4 and resid 196 and name N)	(segid 3A4 and resid 197 and name C)	4.69	0.04	0.04
	assign (segid 3A4 and resid 196 and name N)	(segid 3A4 and resid 197 and name CA)	4.21	0.07	0.07
	assign (segid 3A4 and resid 196 and name N)	(segid 3A4 and resid 197 and name CB)	4.91	0.13	0.13
	assign (segid 3A4 and resid 196 and name N)	(segid 3A4 and resid 197 and name CG)	6.34	0.13	0.13
5	assign (segid 3A4 and resid 196 and name N)	(segid 3A4 and resid 197 and name N)	2.82	0.07	0.08
	assign (segid 3A4 and resid 196 and name N)	(segid 3A4 and resid 197 and name O)	5.75	0.05	0.04
	assign (segid 3A4 and resid 196 and name N)	(segid 3A4 and resid 198 and name C)	5.68	0.07	0.06
	assign (segid 3A4 and resid 196 and name N)	(segid 3A4 and resid 198 and name CA)	5.37	0.07	0.08
	assign (segid 3A4 and resid 196 and name N)	(segid 3A4 and resid 198 and name CB)	5.51	0.15	0.14
10	assign (segid 3A4 and resid 196 and name N)	(segid 3A4 and resid 198 and name CG)	6.08	0.20	0.20
	assign (segid 3A4 and resid 196 and name N)	(segid 3A4 and resid 198 and name N)	4.35	0.04	0.04
	assign (segid 3A4 and resid 196 and name N)	(segid 3A4 and resid 198 and name O)	6.87	0.08	0.09
	assign (segid 3A4 and resid 196 and name N)	(segid 3A4 and resid 199 and name C)	6.57	0.20	0.19
	assign (segid 3A4 and resid 196 and name N)	(segid 3A4 and resid 199 and name CA)	5.60	0.13	0.12
15	assign (segid 3A4 and resid 196 and name N)	(segid 3A4 and resid 199 and name CB)	4.96	0.19	0.20
	assign (segid 3A4 and resid 196 and name N)	(segid 3A4 and resid 199 and name N)	4.85	0.09	0.09
	assign (segid 3A4 and resid 196 and name N)	(segid 3A4 and resid 200 and name N)	6.34	0.28	0.28
	assign (segid 3A4 and resid 196 and name N)	(segid 3A4 and resid 196 and name CB)	3.31	0.08	0.08
	assign (segid 3A4 and resid 196 and name O)	(segid 3A4 and resid 196 and name C)	2.91	0.15	0.15
20	assign (segid 3A4 and resid 196 and name O)	(segid 3A4 and resid 197 and name C)	2.79	0.02	0.02
	assign (segid 3A4 and resid 196 and name O)	(segid 3A4 and resid 197 and name CA)	4.26	0.03	0.04
	assign (segid 3A4 and resid 196 and name O)	(segid 3A4 and resid 197 and name CB)	5.26	0.05	0.06
	assign (segid 3A4 and resid 196 and name O)	(segid 3A4 and resid 197 and name CG)	2.25	0.01	0.02
	assign (segid 3A4 and resid 196 and name O)	(segid 3A4 and resid 197 and name N)	3.34	0.13	0.14
25	assign (segid 3A4 and resid 196 and name O)	(segid 3A4 and resid 197 and name O)	4.11	0.40	0.41
	assign (segid 3A4 and resid 196 and name O)	(segid 3A4 and resid 198 and name C)	4.33	0.35	0.35
	assign (segid 3A4 and resid 196 and name O)	(segid 3A4 and resid 198 and name CA)	5.35	0.40	0.41
	assign (segid 3A4 and resid 196 and name O)	(segid 3A4 and resid 198 and name CB)	6.28	0.38	0.38
	assign (segid 3A4 and resid 196 and name O)	(segid 3A4 and resid 198 and name CG)	3.39	0.28	0.28
30	assign (segid 3A4 and resid 196 and name O)	(segid 3A4 and resid 198 and name N)	5.02	0.41	0.42
	assign (segid 3A4 and resid 196 and name O)	(segid 3A4 and resid 198 and name O)	4.13	0.44	0.44
	assign (segid 3A4 and resid 196 and name O)	(segid 3A4 and resid 199 and name C)	3.90	0.39	0.38
	assign (segid 3A4 and resid 196 and name O)	(segid 3A4 and resid 199 and name CA)	3.72	0.34	0.34
	assign (segid 3A4 and resid 196 and name O)	(segid 3A4 and resid 199 and name CB)	3.40	0.42	0.41
35	assign (segid 3A4 and resid 196 and name O)	(segid 3A4 and resid 199 and name N)	5.32	0.46	0.46
	assign (segid 3A4 and resid 196 and name O)	(segid 3A4 and resid 199 and name O)	5.48	0.44	0.43
	assign (segid 3A4 and resid 196 and name O)	(segid 3A4 and resid 200 and name C)	4.35	0.45	0.45
	assign (segid 3A4 and resid 196 and name O)	(segid 3A4 and resid 200 and name CA)	3.42	0.47	0.47
	assign (segid 3A4 and resid 196 and name O)	(segid 3A4 and resid 200 and name N)	6.61	0.44	0.45
40	assign (segid 3A4 and resid 196 and name O)	(segid 3A4 and resid 200 and name O)	6.75	0.38	0.37
	assign (segid 3A4 and resid 196 and name O)	(segid 3A4 and resid 201 and name CA)	6.91	0.35	0.35
	assign (segid 3A4 and resid 196 and name O)	(segid 3A4 and resid 201 and name CB)	5.43	0.39	0.40
	assign (segid 3A4 and resid 196 and name O)	(segid 3A4 and resid 201 and name N)	2.51	0.03	0.02
	assign (segid 3A4 and resid 197 and name C)	(segid 3A4 and resid 197 and name CG)	2.96	0.08	0.07
45	assign (segid 3A4 and resid 197 and name C)	(segid 3A4 and resid 197 and name O)	1.24	0.01	0.01
	assign (segid 3A4 and resid 197 and name C)	(segid 3A4 and resid 198 and name C)	3.10	0.06	0.06
	assign (segid 3A4 and resid 197 and name C)	(segid 3A4 and resid 198 and name CA)	2.44	0.01	0.02
	assign (segid 3A4 and resid 197 and name C)	(segid 3A4 and resid 198 and name CB)	3.71	0.02	0.02
	assign (segid 3A4 and resid 197 and name C)	(segid 3A4 and resid 198 and name CG)	4.22	0.08	0.08
50	assign (segid 3A4 and resid 197 and name C)	(segid 3A4 and resid 198 and name N)	1.33	0.01	0.01
	assign (segid 3A4 and resid 197 and name C)	(segid 3A4 and resid 198 and name O)	3.93	0.12	0.12
	assign (segid 3A4 and resid 197 and name C)	(segid 3A4 and resid 199 and name C)	4.78	0.19	0.19
	assign (segid 3A4 and resid 197 and name C)	(segid 3A4 and resid 199 and name CA)	4.58	0.13	0.12
	assign (segid 3A4 and resid 197 and name C)	(segid 3A4 and resid 199 and name CB)	5.24	0.16	0.16
55	assign (segid 3A4 and resid 197 and name C)	(segid 3A4 and resid 199 and name N)	3.39	0.11	0.11
	assign (segid 3A4 and resid 197 and name C)	(segid 3A4 and resid 199 and name O)	5.89	0.17	0.17
	assign (segid 3A4 and resid 197 and name C)	(segid 3A4 and resid 200 and name C)	5.26	0.35	0.35
	assign (segid 3A4 and resid 197 and name C)	(segid 3A4 and resid 200 and name CA)	4.87	0.35	0.35
	assign (segid 3A4 and resid 197 and name C)	(segid 3A4 and resid 200 and name N)	4.08	0.30	0.30
60	assign (segid 3A4 and resid 197 and name C)	(segid 3A4 and resid 200 and name O)	6.46	0.34	0.35
	assign (segid 3A4 and resid 197 and name C)	(segid 3A4 and resid 201 and name C)	6.53	0.29	0.29
	assign (segid 3A4 and resid 197 and name C)	(segid 3A4 and resid 201 and name CA)	5.47	0.35	0.34
	assign (segid 3A4 and resid 197 and name C)	(segid 3A4 and resid 201 and name CB)	5.03	0.37	0.37
	assign (segid 3A4 and resid 197 and name C)	(segid 3A4 and resid 201 and name N)	4.57	0.34	0.34
65	assign (segid 3A4 and resid 197 and name C)	(segid 3A4 and resid 202 and name N)	7.61	0.15	0.15
	assign (segid 3A4 and resid 197 and name C)	(segid 3A4 and resid 202 and name O)	6.37	0.24	0.25
	assign (segid 3A4 and resid 197 and name CA)	(segid 3A4 and resid 197 and name C)	1.52	0.01	0.01
	assign (segid 3A4 and resid 197 and name CA)	(segid 3A4 and resid 197 and name CB)	1.54	0.02	0.01
	assign (segid 3A4 and resid 197 and name CA)	(segid 3A4 and resid 197 and name CG)	2.54	0.01	0.01
70	assign (segid 3A4 and resid 197 and name CA)	(segid 3A4 and resid 197 and name O)	2.40	0.02	0.01
	assign (segid 3A4 and resid 197 and name CA)	(segid 3A4 and resid 198 and name C)	4.50	0.07	0.07
	assign (segid 3A4 and resid 197 and name CA)	(segid 3A4 and resid 198 and name CA)	3.81	0.01	0.02
	assign (segid 3A4 and resid 197 and name CA)	(segid 3A4 and resid 198 and name CB)	4.86	0.04	0.04
	assign (segid 3A4 and resid 197 and name CA)	(segid 3A4 and resid 198 and name CG)	5.15	0.09	0.09
75	assign (segid 3A4 and resid 197 and name CA)	(segid 3A4 and resid 198 and name N)	2.44	0.01	0.02
	assign (segid 3A4 and resid 197 and name CA)	(segid 3A4 and resid 198 and name O)	5.40	0.12	0.12
	assign (segid 3A4 and resid 197 and name CA)	(segid 3A4 and resid 199 and name C)	5.82	0.25	0.25
	assign (segid 3A4 and resid 197 and name CA)	(segid 3A4 and resid 199 and name CA)	5.61	0.16	0.16
80	assign (segid 3A4 and resid 197 and name CA)	(segid 3A4 and resid 199 and name CB)	5.94	0.21	0.21
	assign (segid 3A4 and resid 197 and name CA)	(segid 3A4 and resid 199 and name N)	4.52	0.14	0.13
	assign (segid 3A4 and resid 197 and name CA)	(segid 3A4 and resid 199 and name O)	6.97	0.24	0.25
	assign (segid 3A4 and resid 197 and name CA)	(segid 3A4 and resid 200 and name C)	6.27	0.44	0.43

	assign (segid 3A4 and resid 197 and name CA)	(segid 3A4 and resid 200 and name CA)	5.65	0.46	0.45
	assign (segid 3A4 and resid 197 and name CA)	(segid 3A4 and resid 200 and name N)	4.98	0.38	0.37
	assign (segid 3A4 and resid 197 and name CA)	(segid 3A4 and resid 201 and name CA)	6.73	0.39	0.40
	assign (segid 3A4 and resid 197 and name CA)	(segid 3A4 and resid 201 and name CB)	6.36	0.39	0.40
5	assign (segid 3A4 and resid 197 and name CA)	(segid 3A4 and resid 201 and name N)	5.75	0.40	0.41
	assign (segid 3A4 and resid 197 and name CA)	(segid 3A4 and resid 202 and name CA)	9.07	0.24	0.23
	assign (segid 3A4 and resid 197 and name CA)	(segid 3A4 and resid 202 and name CB)	9.02	0.14	0.14
	assign (segid 3A4 and resid 197 and name CA)	(segid 3A4 and resid 203 and name CA)	10.47	0.33	0.32
	assign (segid 3A4 and resid 197 and name CA)	(segid 3A4 and resid 203 and name CB)	10.03	0.36	0.37
10	assign (segid 3A4 and resid 197 and name CA)	(segid 3A4 and resid 204 and name CA)	11.22	0.39	0.38
	assign (segid 3A4 and resid 197 and name CA)	(segid 3A4 and resid 204 and name CB)	10.47	0.34	0.34
	assign (segid 3A4 and resid 197 and name CA)	(segid 3A4 and resid 205 and name CA)	12.72	0.37	0.36
	assign (segid 3A4 and resid 197 and name CA)	(segid 3A4 and resid 205 and name CB)	12.18	0.37	0.38
	assign (segid 3A4 and resid 197 and name CA)	(segid 3A4 and resid 206 and name CA)	14.85	0.28	0.29
	assign (segid 3A4 and resid 197 and name CA)	(segid 3A4 and resid 206 and name CB)	14.57	0.27	0.28
15	assign (segid 3A4 and resid 197 and name CA)	(segid 3A4 and resid 207 and name CA)	16.32	0.43	0.42
	assign (segid 3A4 and resid 197 and name CA)	(segid 3A4 and resid 207 and name CB)	15.79	0.52	0.52
	assign (segid 3A4 and resid 197 and name CA)	(segid 3A4 and resid 219 and name CA)	16.55	0.44	0.43
	assign (segid 3A4 and resid 197 and name CA)	(segid 3A4 and resid 219 and name CB)	15.31	0.44	0.45
20	assign (segid 3A4 and resid 197 and name CA)	(segid 3A4 and resid 220 and name CA)	15.79	0.56	0.57
	assign (segid 3A4 and resid 197 and name CA)	(segid 3A4 and resid 220 and name CB)	15.50	0.69	0.69
	assign (segid 3A4 and resid 197 and name CA)	(segid 3A4 and resid 221 and name CA)	13.04	0.56	0.57
	assign (segid 3A4 and resid 197 and name CA)	(segid 3A4 and resid 221 and name CB)	11.72	0.56	0.56
	assign (segid 3A4 and resid 197 and name CA)	(segid 3A4 and resid 222 and name CA)	15.59	0.62	0.62
25	assign (segid 3A4 and resid 197 and name CA)	(segid 3A4 and resid 222 and name CB)	16.32	0.62	0.62
	assign (segid 3A4 and resid 197 and name CA)	(segid 3A4 and resid 223 and name CA)	18.25	0.60	0.59
	assign (segid 3A4 and resid 197 and name CA)	(segid 3A4 and resid 223 and name CB)	18.77	0.60	0.61
	assign (segid 3A4 and resid 197 and name CA)	(segid 3A4 and resid 224 and name CA)	16.63	0.67	0.67
	assign (segid 3A4 and resid 197 and name CA)	(segid 3A4 and resid 224 and name CB)	15.52	0.61	0.60
30	assign (segid 3A4 and resid 197 and name CA)	(segid 3A4 and resid 225 and name CA)	15.83	1.03	1.03
	assign (segid 3A4 and resid 197 and name CA)	(segid 3A4 and resid 225 and name CB)	15.05	1.05	1.06
	assign (segid 3A4 and resid 197 and name CA)	(segid 3A4 and resid 240 and name CA)	17.02	0.61	0.61
	assign (segid 3A4 and resid 197 and name CA)	(segid 3A4 and resid 240 and name CB)	17.50	0.57	0.58
	assign (segid 3A4 and resid 197 and name CA)	(segid 3A4 and resid 241 and name CA)	13.45	0.72	0.73
	assign (segid 3A4 and resid 197 and name CA)	(segid 3A4 and resid 241 and name CB)	13.15	0.92	0.91
35	assign (segid 3A4 and resid 197 and name CA)	(segid 3A4 and resid 242 and name CA)	13.15	0.51	0.51
	assign (segid 3A4 and resid 197 and name CA)	(segid 3A4 and resid 242 and name CB)	14.14	0.56	0.55
	assign (segid 3A4 and resid 197 and name CA)	(segid 3A4 and resid 243 and name CA)	14.94	0.38	0.37
	assign (segid 3A4 and resid 197 and name CA)	(segid 3A4 and resid 243 and name CB)	16.34	0.37	0.37
	assign (segid 3A4 and resid 197 and name CA)	(segid 3A4 and resid 244 and name CA)	12.96	0.39	0.40
40	assign (segid 3A4 and resid 197 and name CA)	(segid 3A4 and resid 244 and name CB)	12.79	0.56	0.57
	assign (segid 3A4 and resid 197 and name CA)	(segid 3A4 and resid 245 and name CA)	9.76	0.30	0.30
	assign (segid 3A4 and resid 197 and name CA)	(segid 3A4 and resid 245 and name CB)	9.24	0.40	0.41
	assign (segid 3A4 and resid 197 and name CA)	(segid 3A4 and resid 246 and name CA)	12.13	0.18	0.17
	assign (segid 3A4 and resid 197 and name CA)	(segid 3A4 and resid 246 and name CB)	13.36	0.18	0.18
45	assign (segid 3A4 and resid 197 and name CA)	(segid 3A4 and resid 247 and name CA)	13.70	0.08	0.07
	assign (segid 3A4 and resid 197 and name CA)	(segid 3A4 and resid 247 and name CB)	14.45	0.15	0.14
	assign (segid 3A4 and resid 197 and name CA)	(segid 3A4 and resid 248 and name CA)	10.84	0.12	0.12
	assign (segid 3A4 and resid 197 and name CA)	(segid 3A4 and resid 248 and name CB)	9.72	0.15	0.15
	assign (segid 3A4 and resid 197 and name CA)	(segid 3A4 and resid 249 and name CA)	10.16	0.63	0.62
50	assign (segid 3A4 and resid 197 and name CA)	(segid 3A4 and resid 250 and name CA)	13.85	0.69	0.68
	assign (segid 3A4 and resid 197 and name CA)	(segid 3A4 and resid 250 and name CB)	14.87	0.54	0.54
	assign (segid 3A4 and resid 197 and name CA)	(segid 3A4 and resid 251 and name CA)	14.38	0.64	0.63
	assign (segid 3A4 and resid 197 and name CA)	(segid 3A4 and resid 251 and name CB)	14.21	0.50	0.50
	assign (segid 3A4 and resid 197 and name CA)	(segid 3A4 and resid 252 and name CA)	12.29	0.94	0.93
55	assign (segid 3A4 and resid 197 and name CA)	(segid 3A4 and resid 252 and name CB)	10.81	0.96	0.95
	assign (segid 3A4 and resid 197 and name CA)	(segid 3A4 and resid 253 and name CA)	13.97	1.04	1.04
	assign (segid 3A4 and resid 197 and name CA)	(segid 3A4 and resid 254 and name CA)	17.27	0.93	0.92
	assign (segid 3A4 and resid 197 and name CA)	(segid 3A4 and resid 255 and name CA)	17.54	1.28	1.28
	assign (segid 3A4 and resid 197 and name CA)	(segid 3A4 and resid 256 and name CA)	16.87	1.19	1.20
60	assign (segid 3A4 and resid 197 and name CA)	(segid 3A4 and resid 197 and name CG)	1.51	0.01	0.01
	assign (segid 3A4 and resid 197 and name CB)	(segid 3A4 and resid 198 and name C)	5.46	0.04	0.05
	assign (segid 3A4 and resid 197 and name CB)	(segid 3A4 and resid 198 and name CB)	4.42	0.02	0.03
	assign (segid 3A4 and resid 197 and name CB)	(segid 3A4 and resid 198 and name CG)	5.21	0.09	0.09
	assign (segid 3A4 and resid 197 and name CB)	(segid 3A4 and resid 198 and name N)	5.05	0.13	0.13
65	assign (segid 3A4 and resid 197 and name CB)	(segid 3A4 and resid 198 and name O)	3.10	0.03	0.04
	assign (segid 3A4 and resid 197 and name CB)	(segid 3A4 and resid 199 and name C)	6.34	0.10	0.10
	assign (segid 3A4 and resid 197 and name CB)	(segid 3A4 and resid 199 and name CA)	7.20	0.23	0.22
	assign (segid 3A4 and resid 197 and name CB)	(segid 3A4 and resid 199 and name CB)	6.91	0.14	0.14
	assign (segid 3A4 and resid 197 and name CB)	(segid 3A4 and resid 199 and name N)	7.30	0.20	0.21
70	assign (segid 3A4 and resid 197 and name CB)	(segid 3A4 and resid 200 and name CA)	5.68	0.11	0.11
	assign (segid 3A4 and resid 197 and name CB)	(segid 3A4 and resid 200 and name N)	7.01	0.47	0.47
	assign (segid 3A4 and resid 197 and name CB)	(segid 3A4 and resid 201 and name CA)	6.40	0.38	0.37
	assign (segid 3A4 and resid 197 and name CB)	(segid 3A4 and resid 201 and name CB)	7.56	0.44	0.45
	assign (segid 3A4 and resid 197 and name CB)	(segid 3A4 and resid 201 and name N)	6.94	0.45	0.45
75	assign (segid 3A4 and resid 197 and name CB)	(segid 3A4 and resid 202 and name CA)	6.79	0.43	0.44
	assign (segid 3A4 and resid 197 and name CB)	(segid 3A4 and resid 202 and name CB)	10.05	0.23	0.23
	assign (segid 3A4 and resid 197 and name CB)	(segid 3A4 and resid 203 and name CA)	10.03	0.12	0.12
	assign (segid 3A4 and resid 197 and name CB)	(segid 3A4 and resid 203 and name CB)	11.73	0.32	0.32
	assign (segid 3A4 and resid 197 and name CB)	(segid 3A4 and resid 203 and name N)	11.39	0.37	0.37
80	assign (segid 3A4 and resid 197 and name CB)	(segid 3A4 and resid 204 and name CA)	12.25	0.43	0.43
	assign (segid 3A4 and resid 197 and name CB)	(segid 3A4 and resid 204 and name CB)	11.41	0.42	0.42
	assign (segid 3A4 and resid 197 and name CB)	(segid 3A4 and resid 205 and name CA)	13.54	0.38	0.38

	assign (segid 3A4 and resid 197 and name CB)	(segid 3A4 and resid 205 and name CB)	12.91	0.38	0.39
	assign (segid 3A4 and resid 197 and name CB)	(segid 3A4 and resid 206 and name CA)	15.90	0.28	0.28
	assign (segid 3A4 and resid 197 and name CB)	(segid 3A4 and resid 206 and name CB)	15.70	0.25	0.25
	assign (segid 3A4 and resid 197 and name CB)	(segid 3A4 and resid 207 and name CA)	17.40	0.46	0.46
	assign (segid 3A4 and resid 197 and name CB)	(segid 3A4 and resid 207 and name CB)	16.92	0.56	0.56
5	assign (segid 3A4 and resid 197 and name CB)	(segid 3A4 and resid 219 and name CA)	16.52	0.47	0.47
	assign (segid 3A4 and resid 197 and name CB)	(segid 3A4 and resid 219 and name CB)	15.27	0.50	0.50
	assign (segid 3A4 and resid 197 and name CB)	(segid 3A4 and resid 220 and name CA)	15.78	0.56	0.56
	assign (segid 3A4 and resid 197 and name CB)	(segid 3A4 and resid 220 and name CB)	15.38	0.67	0.66
10	assign (segid 3A4 and resid 197 and name CB)	(segid 3A4 and resid 221 and name CA)	13.31	0.57	0.57
	assign (segid 3A4 and resid 197 and name CB)	(segid 3A4 and resid 221 and name CB)	12.00	0.59	0.58
	assign (segid 3A4 and resid 197 and name CB)	(segid 3A4 and resid 222 and name CA)	16.04	0.61	0.62
	assign (segid 3A4 and resid 197 and name CB)	(segid 3A4 and resid 222 and name CB)	16.73	0.61	0.61
	assign (segid 3A4 and resid 197 and name CB)	(segid 3A4 and resid 223 and name CA)	18.60	0.58	0.59
15	assign (segid 3A4 and resid 197 and name CB)	(segid 3A4 and resid 224 and name CA)	17.08	0.69	0.69
	assign (segid 3A4 and resid 197 and name CB)	(segid 3A4 and resid 224 and name CB)	15.91	0.62	0.63
	assign (segid 3A4 and resid 197 and name CB)	(segid 3A4 and resid 225 and name CA)	16.57	1.03	1.03
	assign (segid 3A4 and resid 197 and name CB)	(segid 3A4 and resid 225 and name CB)	15.83	1.07	1.06
	assign (segid 3A4 and resid 197 and name CB)	(segid 3A4 and resid 240 and name CA)	17.95	0.62	0.61
20	assign (segid 3A4 and resid 197 and name CB)	(segid 3A4 and resid 240 and name CB)	18.43	0.58	0.57
	assign (segid 3A4 and resid 197 and name CB)	(segid 3A4 and resid 241 and name CA)	14.46	0.75	0.76
	assign (segid 3A4 and resid 197 and name CB)	(segid 3A4 and resid 241 and name CB)	14.26	0.95	0.95
	assign (segid 3A4 and resid 197 and name CB)	(segid 3A4 and resid 242 and name CA)	13.98	0.48	0.47
	assign (segid 3A4 and resid 197 and name CB)	(segid 3A4 and resid 242 and name CB)	14.98	0.48	0.48
25	assign (segid 3A4 and resid 197 and name CB)	(segid 3A4 and resid 243 and name CA)	15.52	0.34	0.33
	assign (segid 3A4 and resid 197 and name CB)	(segid 3A4 and resid 243 and name CB)	16.93	0.34	0.34
	assign (segid 3A4 and resid 197 and name CB)	(segid 3A4 and resid 244 and name CA)	13.53	0.41	0.40
	assign (segid 3A4 and resid 197 and name CB)	(segid 3A4 and resid 244 and name CB)	13.47	0.57	0.57
	assign (segid 3A4 and resid 197 and name CB)	(segid 3A4 and resid 245 and name CA)	10.25	0.36	0.36
30	assign (segid 3A4 and resid 197 and name CB)	(segid 3A4 and resid 245 and name CB)	9.87	0.48	0.48
	assign (segid 3A4 and resid 197 and name CB)	(segid 3A4 and resid 246 and name CA)	12.30	0.14	0.13
	assign (segid 3A4 and resid 197 and name CB)	(segid 3A4 and resid 246 and name CB)	13.59	0.17	0.16
	assign (segid 3A4 and resid 197 and name CB)	(segid 3A4 and resid 247 and name CA)	13.70	0.18	0.19
	assign (segid 3A4 and resid 197 and name CB)	(segid 3A4 and resid 247 and name CB)	14.54	0.23	0.23
35	assign (segid 3A4 and resid 197 and name CB)	(segid 3A4 and resid 248 and name CA)	10.70	0.20	0.20
	assign (segid 3A4 and resid 197 and name CB)	(segid 3A4 and resid 248 and name CB)	9.70	0.25	0.25
	assign (segid 3A4 and resid 197 and name CB)	(segid 3A4 and resid 249 and name CA)	9.74	0.58	0.58
	assign (segid 3A4 and resid 197 and name CB)	(segid 3A4 and resid 250 and name CA)	13.35	0.73	0.72
	assign (segid 3A4 and resid 197 and name CB)	(segid 3A4 and resid 250 and name CB)	14.47	0.59	0.60
40	assign (segid 3A4 and resid 197 and name CB)	(segid 3A4 and resid 251 and name CA)	13.78	0.69	0.69
	assign (segid 3A4 and resid 197 and name CB)	(segid 3A4 and resid 251 and name CB)	13.70	0.56	0.56
	assign (segid 3A4 and resid 197 and name CB)	(segid 3A4 and resid 252 and name CA)	11.39	0.98	0.98
	assign (segid 3A4 and resid 197 and name CB)	(segid 3A4 and resid 252 and name CB)	9.90	0.99	0.99
	assign (segid 3A4 and resid 197 and name CB)	(segid 3A4 and resid 253 and name CA)	12.98	1.11	1.10
45	assign (segid 3A4 and resid 197 and name CB)	(segid 3A4 and resid 254 and name CA)	16.37	1.02	1.02
	assign (segid 3A4 and resid 197 and name CB)	(segid 3A4 and resid 255 and name CA)	16.56	1.38	1.38
	assign (segid 3A4 and resid 197 and name CB)	(segid 3A4 and resid 256 and name CA)	15.66	1.29	1.30
	assign (segid 3A4 and resid 197 and name CG)	(segid 3A4 and resid 198 and name C)	5.76	0.08	0.09
	assign (segid 3A4 and resid 197 and name CG)	(segid 3A4 and resid 198 and name CA)	4.67	0.12	0.12
50	assign (segid 3A4 and resid 197 and name CG)	(segid 3A4 and resid 198 and name CB)	5.56	0.19	0.19
	assign (segid 3A4 and resid 197 and name CG)	(segid 3A4 and resid 198 and name CG)	5.24	0.24	0.24
	assign (segid 3A4 and resid 197 and name CG)	(segid 3A4 and resid 198 and name N)	3.66	0.10	0.10
	assign (segid 3A4 and resid 197 and name CG)	(segid 3A4 and resid 198 and name O)	6.42	0.12	0.11
	assign (segid 3A4 and resid 197 and name CG)	(segid 3A4 and resid 199 and name CA)	7.50	0.15	0.16
55	assign (segid 3A4 and resid 197 and name CG)	(segid 3A4 and resid 199 and name N)	6.27	0.14	0.15
	assign (segid 3A4 and resid 197 and name CG)	(segid 3A4 and resid 200 and name N)	6.75	0.36	0.36
	assign (segid 3A4 and resid 197 and name CG)	(segid 3A4 and resid 201 and name CA)	7.06	0.51	0.52
	assign (segid 3A4 and resid 197 and name CG)	(segid 3A4 and resid 201 and name CB)	6.28	0.49	0.50
	assign (segid 3A4 and resid 197 and name CG)	(segid 3A4 and resid 201 and name N)	6.53	0.49	0.48
60	assign (segid 3A4 and resid 197 and name N)	(segid 3A4 and resid 197 and name C)	2.46	0.02	0.01
	assign (segid 3A4 and resid 197 and name N)	(segid 3A4 and resid 197 and name CA)	1.46	0.01	0.00
	assign (segid 3A4 and resid 197 and name N)	(segid 3A4 and resid 197 and name CB)	2.44	0.01	0.02
	assign (segid 3A4 and resid 197 and name N)	(segid 3A4 and resid 197 and name CG)	3.79	0.01	0.02
	assign (segid 3A4 and resid 197 and name N)	(segid 3A4 and resid 197 and name O)	3.47	0.02	0.03
65	assign (segid 3A4 and resid 197 and name N)	(segid 3A4 and resid 198 and name C)	4.80	0.09	0.08
	assign (segid 3A4 and resid 197 and name N)	(segid 3A4 and resid 198 and name CA)	4.26	0.04	0.04
	assign (segid 3A4 and resid 197 and name N)	(segid 3A4 and resid 198 and name CB)	5.04	0.05	0.05
	assign (segid 3A4 and resid 197 and name N)	(segid 3A4 and resid 198 and name CG)	5.46	0.11	0.12
	assign (segid 3A4 and resid 197 and name N)	(segid 3A4 and resid 198 and name N)	2.85	0.04	0.05
70	assign (segid 3A4 and resid 197 and name N)	(segid 3A4 and resid 198 and name O)	5.86	0.12	0.13
	assign (segid 3A4 and resid 197 and name N)	(segid 3A4 and resid 199 and name C)	5.89	0.25	0.26
	assign (segid 3A4 and resid 197 and name N)	(segid 3A4 and resid 199 and name CA)	5.43	0.16	0.17
	assign (segid 3A4 and resid 197 and name N)	(segid 3A4 and resid 199 and name CB)	5.41	0.23	0.22
	assign (segid 3A4 and resid 197 and name N)	(segid 3A4 and resid 199 and name N)	4.44	0.15	0.14
75	assign (segid 3A4 and resid 197 and name N)	(segid 3A4 and resid 199 and name O)	7.10	0.25	0.25
	assign (segid 3A4 and resid 197 and name N)	(segid 3A4 and resid 200 and name C)	6.94	0.41	0.40
	assign (segid 3A4 and resid 197 and name N)	(segid 3A4 and resid 200 and name CA)	6.07	0.43	0.43
	assign (segid 3A4 and resid 197 and name N)	(segid 3A4 and resid 200 and name N)	5.20	0.37	0.37
	assign (segid 3A4 and resid 197 and name N)	(segid 3A4 and resid 201 and name N)	6.57	0.35	0.36
80	assign (segid 3A4 and resid 197 and name O)	(segid 3A4 and resid 197 and name CB)	3.35	0.06	0.07
	assign (segid 3A4 and resid 197 and name O)	(segid 3A4 and resid 197 and name CG)	3.34	0.11	0.12
	assign (segid 3A4 and resid 197 and name O)	(segid 3A4 and resid 198 and name C)	3.05	0.08	0.08
	assign (segid 3A4 and resid 197 and name O)	(segid 3A4 and resid 198 and name CA)	2.77	0.03	0.03

	assign (segid 3A4 and resid 197 and name O) (segid 3A4 and resid 198 and name CB)	4.26	0.03	0.03
	assign (segid 3A4 and resid 197 and name O) (segid 3A4 and resid 198 and name CG)	4.86	0.07	0.08
	assign (segid 3A4 and resid 197 and name O) (segid 3A4 and resid 198 and name N)	2.25	0.02	0.01
	assign (segid 3A4 and resid 197 and name O) (segid 3A4 and resid 198 and name O)	3.52	0.16	0.17
5	assign (segid 3A4 and resid 197 and name O) (segid 3A4 and resid 199 and name C)	4.36	0.18	0.19
	assign (segid 3A4 and resid 197 and name O) (segid 3A4 and resid 199 and name CA)	4.52	0.10	0.11
	assign (segid 3A4 and resid 197 and name O) (segid 3A4 and resid 199 and name CB)	5.40	0.12	0.12
	assign (segid 3A4 and resid 197 and name O) (segid 3A4 and resid 199 and name N)	3.55	0.09	0.09
	assign (segid 3A4 and resid 197 and name O) (segid 3A4 and resid 199 and name O)	5.34	0.19	0.19
10	assign (segid 3A4 and resid 197 and name O) (segid 3A4 and resid 200 and name C)	4.22	0.36	0.36
	assign (segid 3A4 and resid 197 and name O) (segid 3A4 and resid 200 and name CA)	4.04	0.33	0.33
	assign (segid 3A4 and resid 197 and name O) (segid 3A4 and resid 200 and name N)	3.52	0.27	0.27
	assign (segid 3A4 and resid 197 and name O) (segid 3A4 and resid 200 and name O)	5.39	0.37	0.36
	assign (segid 3A4 and resid 197 and name O) (segid 3A4 and resid 201 and name C)	5.53	0.35	0.35
15	assign (segid 3A4 and resid 197 and name O) (segid 3A4 and resid 201 and name CA)	4.36	0.39	0.39
	assign (segid 3A4 and resid 197 and name O) (segid 3A4 and resid 201 and name CB)	4.04	0.40	0.39
	assign (segid 3A4 and resid 197 and name O) (segid 3A4 and resid 201 and name N)	3.47	0.38	0.38
	assign (segid 3A4 and resid 197 and name O) (segid 3A4 and resid 201 and name O)	6.65	0.36	0.36
	assign (segid 3A4 and resid 197 and name O) (segid 3A4 and resid 202 and name CA)	6.91	0.31	0.32
20	assign (segid 3A4 and resid 197 and name O) (segid 3A4 and resid 202 and name CB)	7.10	0.24	0.23
	assign (segid 3A4 and resid 197 and name O) (segid 3A4 and resid 202 and name N)	5.55	0.32	0.31
	assign (segid 3A4 and resid 198 and name C) (segid 3A4 and resid 198 and name CB)	2.51	0.01	0.01
	assign (segid 3A4 and resid 198 and name C) (segid 3A4 and resid 198 and name CG)	3.87	0.03	0.03
	assign (segid 3A4 and resid 198 and name C) (segid 3A4 and resid 198 and name O)	1.24	0.01	0.00
25	assign (segid 3A4 and resid 198 and name C) (segid 3A4 and resid 199 and name C)	3.01	0.03	0.03
	assign (segid 3A4 and resid 198 and name C) (segid 3A4 and resid 199 and name CA)	2.44	0.01	0.01
	assign (segid 3A4 and resid 198 and name C) (segid 3A4 and resid 199 and name CB)	3.71	0.03	0.03
	assign (segid 3A4 and resid 198 and name C) (segid 3A4 and resid 199 and name N)	1.33	0.01	0.01
	assign (segid 3A4 and resid 198 and name C) (segid 3A4 and resid 199 and name O)	3.86	0.08	0.08
30	assign (segid 3A4 and resid 198 and name C) (segid 3A4 and resid 200 and name C)	4.49	0.07	0.07
	assign (segid 3A4 and resid 198 and name C) (segid 3A4 and resid 200 and name CA)	4.40	0.09	0.09
	assign (segid 3A4 and resid 198 and name C) (segid 3A4 and resid 200 and name N)	3.23	0.10	0.10
	assign (segid 3A4 and resid 198 and name C) (segid 3A4 and resid 200 and name O)	5.58	0.10	0.10
	assign (segid 3A4 and resid 198 and name C) (segid 3A4 and resid 201 and name C)	4.84	0.08	0.08
35	assign (segid 3A4 and resid 198 and name C) (segid 3A4 and resid 201 and name CA)	4.46	0.07	0.07
	assign (segid 3A4 and resid 198 and name C) (segid 3A4 and resid 201 and name CB)	4.21	0.11	0.12
	assign (segid 3A4 and resid 198 and name C) (segid 3A4 and resid 201 and name N)	3.74	0.06	0.06
	assign (segid 3A4 and resid 198 and name C) (segid 3A4 and resid 201 and name O)	6.05	0.08	0.08
	assign (segid 3A4 and resid 198 and name C) (segid 3A4 and resid 202 and name C)	6.21	0.12	0.12
40	assign (segid 3A4 and resid 198 and name C) (segid 3A4 and resid 202 and name CA)	5.10	0.11	0.12
	assign (segid 3A4 and resid 198 and name C) (segid 3A4 and resid 202 and name CB)	4.74	0.10	0.09
	assign (segid 3A4 and resid 198 and name C) (segid 3A4 and resid 202 and name CG1)	6.12	0.09	0.10
	assign (segid 3A4 and resid 198 and name C) (segid 3A4 and resid 202 and name N)	4.14	0.10	0.10
	assign (segid 3A4 and resid 198 and name C) (segid 3A4 and resid 202 and name O)	7.37	0.12	0.13
45	assign (segid 3A4 and resid 198 and name C) (segid 3A4 and resid 203 and name CA)	7.35	0.12	0.12
	assign (segid 3A4 and resid 198 and name C) (segid 3A4 and resid 203 and name CB)	7.36	0.12	0.13
	assign (segid 3A4 and resid 198 and name C) (segid 3A4 and resid 203 and name N)	6.07	0.13	0.13
	assign (segid 3A4 and resid 198 and name C) (segid 3A4 and resid 204 and name N)	7.87	0.06	0.06
	assign (segid 3A4 and resid 198 and name C) (segid 3A4 and resid 245 and name C)	7.10	0.40	0.40
50	assign (segid 3A4 and resid 198 and name C) (segid 3A4 and resid 245 and name CA)	6.20	0.33	0.34
	assign (segid 3A4 and resid 198 and name C) (segid 3A4 and resid 245 and name CB)	5.89	0.39	0.38
	assign (segid 3A4 and resid 198 and name C) (segid 3A4 and resid 245 and name N)	7.08	0.33	0.33
	assign (segid 3A4 and resid 198 and name C) (segid 3A4 and resid 245 and name O)	6.91	0.48	0.48
	assign (segid 3A4 and resid 198 and name C) (segid 3A4 and resid 248 and name CB)	6.77	0.17	0.16
55	assign (segid 3A4 and resid 198 and name CA) (segid 3A4 and resid 198 and name CB)	1.52	0.00	0.01
	assign (segid 3A4 and resid 198 and name CA) (segid 3A4 and resid 198 and name CG)	1.54	0.01	0.01
	assign (segid 3A4 and resid 198 and name CA) (segid 3A4 and resid 198 and name O)	2.41	0.02	0.01
	assign (segid 3A4 and resid 198 and name CA) (segid 3A4 and resid 199 and name C)	4.43	0.04	0.03
60	assign (segid 3A4 and resid 198 and name CA) (segid 3A4 and resid 199 and name CA)	3.80	0.02	0.03
	assign (segid 3A4 and resid 198 and name CA) (segid 3A4 and resid 199 and name CB)	4.83	0.05	0.05
	assign (segid 3A4 and resid 198 and name CA) (segid 3A4 and resid 199 and name N)	2.42	0.02	0.02
	assign (segid 3A4 and resid 198 and name CA) (segid 3A4 and resid 199 and name O)	5.34	0.07	0.07
	assign (segid 3A4 and resid 198 and name CA) (segid 3A4 and resid 200 and name C)	5.51	0.12	0.12
65	assign (segid 3A4 and resid 198 and name CA) (segid 3A4 and resid 200 and name CA)	5.45	0.12	0.13
	assign (segid 3A4 and resid 198 and name CA) (segid 3A4 and resid 200 and name N)	4.38	0.13	0.12
	assign (segid 3A4 and resid 198 and name CA) (segid 3A4 and resid 200 and name O)	6.63	0.12	0.13
	assign (segid 3A4 and resid 198 and name CA) (segid 3A4 and resid 201 and name C)	5.75	0.13	0.13
	assign (segid 3A4 and resid 198 and name CA) (segid 3A4 and resid 201 and name CB)	5.14	0.15	0.14
70	assign (segid 3A4 and resid 198 and name CA) (segid 3A4 and resid 201 and name N)	4.47	0.22	0.23
	assign (segid 3A4 and resid 198 and name CA) (segid 3A4 and resid 201 and name O)	4.57	0.11	0.11
	assign (segid 3A4 and resid 198 and name CA) (segid 3A4 and resid 201 and name N)	6.93	0.13	0.13
	assign (segid 3A4 and resid 198 and name CA) (segid 3A4 and resid 202 and name C)	7.49	0.16	0.17
	assign (segid 3A4 and resid 198 and name CA) (segid 3A4 and resid 202 and name CA)	6.28	0.17	0.17
75	assign (segid 3A4 and resid 198 and name CA) (segid 3A4 and resid 202 and name CB)	5.97	0.17	0.17
	assign (segid 3A4 and resid 198 and name CA) (segid 3A4 and resid 202 and name CG1)	7.36	0.16	0.16
	assign (segid 3A4 and resid 198 and name CA) (segid 3A4 and resid 202 and name N)	5.24	0.15	0.15
	assign (segid 3A4 and resid 198 and name CA) (segid 3A4 and resid 203 and name CA)	8.75	0.15	0.14
80	assign (segid 3A4 and resid 198 and name CA) (segid 3A4 and resid 203 and name CB)	8.79	0.14	0.14
	assign (segid 3A4 and resid 198 and name CA) (segid 3A4 and resid 203 and name N)	7.45	0.16	0.16
	assign (segid 3A4 and resid 198 and name CA) (segid 3A4 and resid 204 and name CA)	9.99	0.10	0.10
	assign (segid 3A4 and resid 198 and name CA) (segid 3A4 and resid 204 and name CB)	9.56	0.22	0.21
	assign (segid 3A4 and resid 198 and name CA) (segid 3A4 and resid 205 and name CA)	10.49	0.15	0.16

assign (segid 3A4 and resid 198 and name CA) (segid 3A4 and resid 205 and name CB) 9.67 0.21 0.21
assign (segid 3A4 and resid 198 and name CA) (segid 3A4 and resid 206 and name CA) 12.47 0.18 0.18
assign (segid 3A4 and resid 198 and name CA) (segid 3A4 and resid 206 and name CB) 12.19 0.20 0.20
assign (segid 3A4 and resid 198 and name CA) (segid 3A4 and resid 207 and name CA) 14.63 0.22 0.22
5 assign (segid 3A4 and resid 198 and name CA) (segid 3A4 and resid 207 and name CB) 14.44 0.33 0.32
assign (segid 3A4 and resid 198 and name CA) (segid 3A4 and resid 219 and name CA) 13.81 0.51 0.51
assign (segid 3A4 and resid 198 and name CA) (segid 3A4 and resid 219 and name CB) 12.75 0.46 0.46
assign (segid 3A4 and resid 198 and name CA) (segid 3A4 and resid 220 and name CA) 12.56 0.68 0.69
assign (segid 3A4 and resid 198 and name CA) (segid 3A4 and resid 220 and name CB) 12.29 0.82 0.82
10 assign (segid 3A4 and resid 198 and name CA) (segid 3A4 and resid 221 and name CA) 9.68 0.63 0.64
assign (segid 3A4 and resid 198 and name CA) (segid 3A4 and resid 221 and name CB) 8.51 0.61 0.61
assign (segid 3A4 and resid 198 and name CA) (segid 3A4 and resid 222 and name CA) 12.44 0.67 0.68
assign (segid 3A4 and resid 198 and name CA) (segid 3A4 and resid 222 and name CB) 13.36 0.67 0.67
assign (segid 3A4 and resid 198 and name CA) (segid 3A4 and resid 223 and name CA) 14.79 0.67 0.67
15 assign (segid 3A4 and resid 198 and name CA) (segid 3A4 and resid 223 and name CB) 15.31 0.68 0.69
assign (segid 3A4 and resid 198 and name CA) (segid 3A4 and resid 224 and name CA) 12.95 0.70 0.71
assign (segid 3A4 and resid 198 and name CA) (segid 3A4 and resid 224 and name CB) 11.81 0.63 0.62
assign (segid 3A4 and resid 198 and name CA) (segid 3A4 and resid 225 and name CA) 12.38 1.08 1.07
assign (segid 3A4 and resid 198 and name CA) (segid 3A4 and resid 225 and name CB) 11.75 1.13 1.13
20 assign (segid 3A4 and resid 198 and name CA) (segid 3A4 and resid 226 and name CA) 16.02 1.09 1.09
assign (segid 3A4 and resid 198 and name CA) (segid 3A4 and resid 240 and name CA) 13.85 0.42 0.42
assign (segid 3A4 and resid 198 and name CA) (segid 3A4 and resid 240 and name CB) 14.46 0.38 0.38
assign (segid 3A4 and resid 198 and name CA) (segid 3A4 and resid 241 and name CA) 10.46 0.55 0.54
assign (segid 3A4 and resid 198 and name CA) (segid 3A4 and resid 241 and name CB) 10.44 0.68 0.68
25 assign (segid 3A4 and resid 198 and name CA) (segid 3A4 and resid 242 and name CA) 10.38 0.46 0.45
assign (segid 3A4 and resid 198 and name CA) (segid 3A4 and resid 242 and name CB) 11.58 0.50 0.50
assign (segid 3A4 and resid 198 and name CA) (segid 3A4 and resid 243 and name CA) 11.65 0.34 0.34
assign (segid 3A4 and resid 198 and name CA) (segid 3A4 and resid 243 and name CB) 12.98 0.32 0.32
assign (segid 3A4 and resid 198 and name CA) (segid 3A4 and resid 244 and name CA) 9.32 0.33 0.34
30 assign (segid 3A4 and resid 198 and name CA) (segid 3A4 and resid 244 and name CB) 9.16 0.50 0.50
assign (segid 3A4 and resid 198 and name CA) (segid 3A4 and resid 245 and name C) 7.01 0.25 0.26
assign (segid 3A4 and resid 198 and name CA) (segid 3A4 and resid 245 and name CA) 6.40 0.27 0.26
assign (segid 3A4 and resid 198 and name CA) (segid 3A4 and resid 245 and name CB) 6.22 0.33 0.32
assign (segid 3A4 and resid 198 and name CA) (segid 3A4 and resid 245 and name O) 6.58 0.35 0.34
35 assign (segid 3A4 and resid 198 and name CA) (segid 3A4 and resid 246 and name CA) 9.17 0.38 0.37
assign (segid 3A4 and resid 198 and name CA) (segid 3A4 and resid 246 and name CB) 10.48 0.37 0.37
assign (segid 3A4 and resid 198 and name CA) (segid 3A4 and resid 247 and name CA) 10.32 0.15 0.15
assign (segid 3A4 and resid 198 and name CA) (segid 3A4 and resid 247 and name CB) 10.91 0.16 0.15
40 assign (segid 3A4 and resid 198 and name CA) (segid 3A4 and resid 248 and name CA) 7.53 0.16 0.15
assign (segid 3A4 and resid 198 and name CA) (segid 3A4 and resid 248 and name CB) 6.27 0.13 0.12
assign (segid 3A4 and resid 198 and name CA) (segid 3A4 and resid 249 and name CA) 7.73 0.75 0.75
assign (segid 3A4 and resid 198 and name CA) (segid 3A4 and resid 250 and name CA) 11.36 0.67 0.67
45 assign (segid 3A4 and resid 198 and name CA) (segid 3A4 and resid 250 and name CB) 12.18 0.53 0.54
assign (segid 3A4 and resid 198 and name CA) (segid 3A4 and resid 251 and name CA) 11.74 0.55 0.54
assign (segid 3A4 and resid 198 and name CA) (segid 3A4 and resid 251 and name CB) 11.35 0.43 0.42
assign (segid 3A4 and resid 198 and name CA) (segid 3A4 and resid 252 and name CA) 10.47 0.82 0.82
50 assign (segid 3A4 and resid 198 and name CA) (segid 3A4 and resid 252 and name CB) 9.14 0.87 0.86
assign (segid 3A4 and resid 198 and name CA) (segid 3A4 and resid 253 and name CA) 12.64 0.91 0.90
assign (segid 3A4 and resid 198 and name CA) (segid 3A4 and resid 254 and name CA) 15.43 0.76 0.76
assign (segid 3A4 and resid 198 and name CA) (segid 3A4 and resid 255 and name CA) 15.78 1.08 1.08
assign (segid 3A4 and resid 198 and name CA) (segid 3A4 and resid 256 and name CA) 15.90 0.87 0.86
55 assign (segid 3A4 and resid 198 and name CA) (segid 3A4 and resid 392 and name CB) 19.34 0.44 0.44
assign (segid 3A4 and resid 198 and name CB) (segid 3A4 and resid 198 and name CG) 1.53 0.00 0.00
assign (segid 3A4 and resid 198 and name CB) (segid 3A4 and resid 199 and name C) 5.42 0.04 0.05
assign (segid 3A4 and resid 198 and name CB) (segid 3A4 and resid 199 and name CA) 4.48 0.06 0.06
assign (segid 3A4 and resid 198 and name CB) (segid 3A4 and resid 199 and name CB) 5.35 0.09 0.08
60 assign (segid 3A4 and resid 198 and name CB) (segid 3A4 and resid 199 and name N) 3.15 0.07 0.06
assign (segid 3A4 and resid 198 and name CB) (segid 3A4 and resid 199 and name O) 6.26 0.09 0.10
assign (segid 3A4 and resid 198 and name CB) (segid 3A4 and resid 200 and name C) 6.87 0.10 0.09
assign (segid 3A4 and resid 198 and name CB) (segid 3A4 and resid 200 and name CA) 6.82 0.11 0.11
assign (segid 3A4 and resid 198 and name CB) (segid 3A4 and resid 200 and name N) 5.63 0.13 0.12
65 assign (segid 3A4 and resid 198 and name CB) (segid 3A4 and resid 201 and name C) 6.75 0.11 0.12
assign (segid 3A4 and resid 198 and name CB) (segid 3A4 and resid 201 and name CA) 6.36 0.13 0.12
assign (segid 3A4 and resid 198 and name CB) (segid 3A4 and resid 201 and name CB) 5.58 0.21 0.22
assign (segid 3A4 and resid 198 and name CB) (segid 3A4 and resid 201 and name N) 5.93 0.08 0.08
70 assign (segid 3A4 and resid 198 and name CB) (segid 3A4 and resid 202 and name CA) 6.87 0.19 0.19
assign (segid 3A4 and resid 198 and name CB) (segid 3A4 and resid 202 and name CB) 6.30 0.24 0.23
assign (segid 3A4 and resid 198 and name CB) (segid 3A4 and resid 202 and name CG1) 7.53 0.24 0.25
assign (segid 3A4 and resid 198 and name CB) (segid 3A4 and resid 202 and name N) 6.08 0.16 0.15
75 assign (segid 3A4 and resid 198 and name CB) (segid 3A4 and resid 203 and name CA) 9.65 0.17 0.17
assign (segid 3A4 and resid 198 and name CB) (segid 3A4 and resid 203 and name CB) 9.79 0.14 0.13
assign (segid 3A4 and resid 198 and name CB) (segid 3A4 and resid 204 and name CA) 11.13 0.13 0.14
assign (segid 3A4 and resid 198 and name CB) (segid 3A4 and resid 204 and name CB) 10.80 0.25 0.26
80 assign (segid 3A4 and resid 198 and name CB) (segid 3A4 and resid 205 and name CA) 11.27 0.17 0.17
assign (segid 3A4 and resid 198 and name CB) (segid 3A4 and resid 205 and name CB) 10.31 0.19 0.20
assign (segid 3A4 and resid 198 and name CB) (segid 3A4 and resid 206 and name CA) 13.09 0.25 0.25
assign (segid 3A4 and resid 198 and name CB) (segid 3A4 and resid 206 and name CB) 12.76 0.26 0.27
assign (segid 3A4 and resid 198 and name CB) (segid 3A4 and resid 207 and name CA) 15.53 0.23 0.24
assign (segid 3A4 and resid 198 and name CB) (segid 3A4 and resid 207 and name CB) 15.45 0.32 0.33
assign (segid 3A4 and resid 198 and name CB) (segid 3A4 and resid 219 and name CA) 13.86 0.56 0.55
assign (segid 3A4 and resid 198 and name CB) (segid 3A4 and resid 219 and name CB) 12.90 0.49 0.50
assign (segid 3A4 and resid 198 and name CB) (segid 3A4 and resid 220 and name CA) 12.22 0.75 0.75
assign (segid 3A4 and resid 198 and name CB) (segid 3A4 and resid 220 and name CB) 11.81 0.88 0.88

assign (segid 3A4 and resid 198 and name CB) (segid 3A4 and resid 221 and name CA) 9.52 0.68 0.69
 assign (segid 3A4 and resid 198 and name CB) (segid 3A4 and resid 221 and name CB) 8.51 0.64 0.65
 assign (segid 3A4 and resid 198 and name CB) (segid 3A4 and resid 222 and name CA) 12.56 0.70 0.70
 assign (segid 3A4 and resid 198 and name CB) (segid 3A4 and resid 222 and name CB) 13.58 0.69 0.68
 5 assign (segid 3A4 and resid 198 and name CB) (segid 3A4 and resid 223 and name CA) 14.55 0.72 0.72
 assign (segid 3A4 and resid 198 and name CB) (segid 3A4 and resid 223 and name CB) 14.99 0.75 0.75
 assign (segid 3A4 and resid 198 and name CB) (segid 3A4 and resid 224 and name CA) 12.47 0.78 0.77
 assign (segid 3A4 and resid 198 and name CB) (segid 3A4 and resid 224 and name CB) 11.22 0.70 0.71
 assign (segid 3A4 and resid 198 and name CB) (segid 3A4 and resid 225 and name CA) 12.24 1.13 1.13
 10 assign (segid 3A4 and resid 198 and name CB) (segid 3A4 and resid 225 and name CB) 11.79 1.17 1.17
 assign (segid 3A4 and resid 198 and name CB) (segid 3A4 and resid 226 and name CA) 15.93 1.11 1.12
 assign (segid 3A4 and resid 198 and name CB) (segid 3A4 and resid 240 and name CA) 13.22 0.45 0.44
 assign (segid 3A4 and resid 198 and name CB) (segid 3A4 and resid 240 and name CB) 13.77 0.38 0.37
 assign (segid 3A4 and resid 198 and name CB) (segid 3A4 and resid 241 and name CA) 10.00 0.57 0.58
 15 assign (segid 3A4 and resid 198 and name CB) (segid 3A4 and resid 241 and name CB) 10.16 0.70 0.70
 assign (segid 3A4 and resid 198 and name CB) (segid 3A4 and resid 242 and name CA) 9.54 0.36 0.36
 assign (segid 3A4 and resid 198 and name CB) (segid 3A4 and resid 242 and name CB) 10.73 0.39 0.40
 assign (segid 3A4 and resid 198 and name CB) (segid 3A4 and resid 243 and name CA) 10.54 0.29 0.29
 assign (segid 3A4 and resid 198 and name CB) (segid 3A4 and resid 243 and name CB) 11.91 0.29 0.28
 20 assign (segid 3A4 and resid 198 and name CB) (segid 3A4 and resid 244 and name CA) 7.04 0.31 0.32
 assign (segid 3A4 and resid 198 and name CB) (segid 3A4 and resid 244 and name CB) 8.39 0.38 0.38
 assign (segid 3A4 and resid 198 and name CB) (segid 3A4 and resid 244 and name CB) 8.44 0.57 0.58
 assign (segid 3A4 and resid 198 and name CB) (segid 3A4 and resid 244 and name O) 6.83 0.28 0.27
 assign (segid 3A4 and resid 198 and name CB) (segid 3A4 and resid 245 and name C) 5.66 0.18 0.19
 25 assign (segid 3A4 and resid 198 and name CB) (segid 3A4 and resid 245 and name CA) 5.25 0.30 0.29
 assign (segid 3A4 and resid 198 and name CB) (segid 3A4 and resid 245 and name CB) 5.18 0.36 0.36
 assign (segid 3A4 and resid 198 and name CB) (segid 3A4 and resid 245 and name N) 6.42 0.36 0.37
 assign (segid 3A4 and resid 198 and name CB) (segid 3A4 and resid 245 and name O) 5.14 0.27 0.26
 assign (segid 3A4 and resid 198 and name CB) (segid 3A4 and resid 246 and name CA) 7.72 0.34 0.33
 30 assign (segid 3A4 and resid 198 and name CB) (segid 3A4 and resid 246 and name CB) 9.06 0.33 0.34
 assign (segid 3A4 and resid 198 and name CB) (segid 3A4 and resid 246 and name N) 6.90 0.21 0.21
 assign (segid 3A4 and resid 198 and name CB) (segid 3A4 and resid 247 and name CA) 8.95 0.09 0.10
 assign (segid 3A4 and resid 198 and name CB) (segid 3A4 and resid 247 and name CB) 9.64 0.17 0.18
 assign (segid 3A4 and resid 198 and name CB) (segid 3A4 and resid 248 and name C) 6.20 0.31 0.31
 35 assign (segid 3A4 and resid 198 and name CB) (segid 3A4 and resid 248 and name CA) 6.32 0.08 0.08
 assign (segid 3A4 and resid 198 and name CB) (segid 3A4 and resid 248 and name CB) 5.18 0.19 0.19
 assign (segid 3A4 and resid 198 and name CB) (segid 3A4 and resid 248 and name N) 6.96 0.06 0.07
 assign (segid 3A4 and resid 198 and name CB) (segid 3A4 and resid 248 and name O) 6.71 0.42 0.41
 assign (segid 3A4 and resid 198 and name CB) (segid 3A4 and resid 249 and name CA) 6.30 0.74 0.74
 40 assign (segid 3A4 and resid 198 and name CB) (segid 3A4 and resid 249 and name N) 5.95 0.50 0.49
 assign (segid 3A4 and resid 198 and name CB) (segid 3A4 and resid 250 and name CA) 9.93 0.65 0.64
 assign (segid 3A4 and resid 198 and name CB) (segid 3A4 and resid 250 and name CB) 10.72 0.52 0.52
 assign (segid 3A4 and resid 198 and name CB) (segid 3A4 and resid 251 and name CA) 10.55 0.49 0.50
 assign (segid 3A4 and resid 198 and name CB) (segid 3A4 and resid 251 and name CB) 10.25 0.38 0.38
 45 assign (segid 3A4 and resid 198 and name CB) (segid 3A4 and resid 252 and name CA) 9.50 0.73 0.73
 assign (segid 3A4 and resid 198 and name CB) (segid 3A4 and resid 252 and name CB) 8.22 0.78 0.77
 assign (segid 3A4 and resid 198 and name CB) (segid 3A4 and resid 253 and name CA) 11.51 0.83 0.82
 assign (segid 3A4 and resid 198 and name CB) (segid 3A4 and resid 254 and name CA) 14.22 0.71 0.70
 assign (segid 3A4 and resid 198 and name CB) (segid 3A4 and resid 255 and name CA) 14.80 0.95 0.95
 50 assign (segid 3A4 and resid 198 and name CB) (segid 3A4 and resid 256 and name CA) 15.10 0.75 0.75
 assign (segid 3A4 and resid 198 and name CB) (segid 3A4 and resid 257 and name CA) 17.46 1.08 1.09
 assign (segid 3A4 and resid 198 and name CB) (segid 3A4 and resid 392 and name CA) 19.36 0.38 0.38
 assign (segid 3A4 and resid 198 and name CB) (segid 3A4 and resid 392 and name CB) 18.14 0.42 0.42
 assign (segid 3A4 and resid 198 and name CB) (segid 3A4 and resid 393 and name CA) 18.73 0.33 0.33
 55 assign (segid 3A4 and resid 198 and name CG) (segid 3A4 and resid 199 and name C) 6.84 0.06 0.05
 assign (segid 3A4 and resid 198 and name CG) (segid 3A4 and resid 199 and name CA) 5.96 0.06 0.06
 assign (segid 3A4 and resid 198 and name CG) (segid 3A4 and resid 199 and name CB) 6.79 0.09 0.09
 assign (segid 3A4 and resid 198 and name CG) (segid 3A4 and resid 199 and name N) 4.58 0.06 0.07
 assign (segid 3A4 and resid 198 and name CG) (segid 3A4 and resid 199 and name O) 7.69 0.10 0.10
 60 assign (segid 3A4 and resid 198 and name CG) (segid 3A4 and resid 200 and name N) 6.89 0.15 0.16
 assign (segid 3A4 and resid 198 and name CG) (segid 3A4 and resid 201 and name C) 7.70 0.18 0.18
 assign (segid 3A4 and resid 198 and name CG) (segid 3A4 and resid 201 and name CA) 7.18 0.20 0.20
 assign (segid 3A4 and resid 198 and name CG) (segid 3A4 and resid 201 and name CB) 6.15 0.28 0.29
 assign (segid 3A4 and resid 198 and name CG) (segid 3A4 and resid 201 and name N) 6.91 0.15 0.14
 65 assign (segid 3A4 and resid 198 and name CG) (segid 3A4 and resid 202 and name CB) 7.55 0.30 0.29
 assign (segid 3A4 and resid 198 and name CG) (segid 3A4 and resid 202 and name N) 7.18 0.22 0.21
 assign (segid 3A4 and resid 198 and name CG) (segid 3A4 and resid 244 and name O) 7.16 0.28 0.28
 assign (segid 3A4 and resid 198 and name CG) (segid 3A4 and resid 245 and name C) 5.98 0.14 0.14
 assign (segid 3A4 and resid 198 and name CG) (segid 3A4 and resid 245 and name CA) 5.90 0.35 0.35
 70 assign (segid 3A4 and resid 198 and name CG) (segid 3A4 and resid 245 and name CB) 6.06 0.44 0.43
 assign (segid 3A4 and resid 198 and name CG) (segid 3A4 and resid 245 and name O) 5.18 0.11 0.11
 assign (segid 3A4 and resid 198 and name CG) (segid 3A4 and resid 246 and name N) 7.20 0.13 0.13
 assign (segid 3A4 and resid 198 and name CG) (segid 3A4 and resid 247 and name C) 7.71 0.14 0.13
 assign (segid 3A4 and resid 198 and name CG) (segid 3A4 and resid 248 and name C) 5.40 0.27 0.27
 75 assign (segid 3A4 and resid 198 and name CG) (segid 3A4 and resid 248 and name CA) 5.80 0.16 0.16
 assign (segid 3A4 and resid 198 and name CG) (segid 3A4 and resid 248 and name CB) 4.84 0.35 0.35
 assign (segid 3A4 and resid 198 and name CG) (segid 3A4 and resid 248 and name N) 6.64 0.14 0.15
 assign (segid 3A4 and resid 198 and name CG) (segid 3A4 and resid 248 and name O) 5.69 0.42 0.42
 assign (segid 3A4 and resid 198 and name CG) (segid 3A4 and resid 249 and name CA) 5.36 0.69 0.69
 80 assign (segid 3A4 and resid 198 and name CG) (segid 3A4 and resid 249 and name N) 5.20 0.40 0.40
 assign (segid 3A4 and resid 198 and name N) (segid 3A4 and resid 198 and name C) 2.49 0.02 0.01
 assign (segid 3A4 and resid 198 and name N) (segid 3A4 and resid 198 and name CA) 1.46 0.01 0.01
 assign (segid 3A4 and resid 198 and name N) (segid 3A4 and resid 198 and name CB) 2.46 0.02 0.02

	assign	(segid 3A4 and resid 198 and name N)	(segid 3A4 and resid 198 and name CG)	3.06	0.08	0.07
	assign	(segid 3A4 and resid 198 and name N)	(segid 3A4 and resid 198 and name O)	3.53	0.05	0.04
	assign	(segid 3A4 and resid 198 and name N)	(segid 3A4 and resid 199 and name C)	4.82	0.10	0.09
	assign	(segid 3A4 and resid 198 and name N)	(segid 3A4 and resid 199 and name CA)	4.24	0.08	0.07
5	assign	(segid 3A4 and resid 198 and name N)	(segid 3A4 and resid 199 and name CB)	4.93	0.13	0.13
	assign	(segid 3A4 and resid 198 and name N)	(segid 3A4 and resid 199 and name N)	2.83	0.07	0.07
	assign	(segid 3A4 and resid 198 and name N)	(segid 3A4 and resid 199 and name O)	5.91	0.06	0.06
	assign	(segid 3A4 and resid 198 and name N)	(segid 3A4 and resid 200 and name C)	5.83	0.21	0.22
	assign	(segid 3A4 and resid 198 and name N)	(segid 3A4 and resid 200 and name CA)	5.50	0.22	0.22
10	assign	(segid 3A4 and resid 198 and name N)	(segid 3A4 and resid 200 and name N)	4.46	0.21	0.20
	assign	(segid 3A4 and resid 198 and name N)	(segid 3A4 and resid 200 and name O)	7.04	0.21	0.20
	assign	(segid 3A4 and resid 198 and name N)	(segid 3A4 and resid 201 and name C)	6.67	0.18	0.18
	assign	(segid 3A4 and resid 198 and name N)	(segid 3A4 and resid 201 and name CA)	5.83	0.23	0.23
	assign	(segid 3A4 and resid 198 and name N)	(segid 3A4 and resid 201 and name CB)	5.26	0.30	0.30
15	assign	(segid 3A4 and resid 198 and name N)	(segid 3A4 and resid 201 and name N)	5.05	0.21	0.20
	assign	(segid 3A4 and resid 198 and name N)	(segid 3A4 and resid 202 and name CA)	7.43	0.15	0.16
	assign	(segid 3A4 and resid 198 and name N)	(segid 3A4 and resid 202 and name CB)	7.18	0.12	0.12
	assign	(segid 3A4 and resid 198 and name N)	(segid 3A4 and resid 202 and name N)	6.30	0.16	0.16
	assign	(segid 3A4 and resid 198 and name N)	(segid 3A4 and resid 245 and name CB)	7.08	0.38	0.37
20	assign	(segid 3A4 and resid 198 and name N)	(segid 3A4 and resid 245 and name O)	7.46	0.21	0.22
	assign	(segid 3A4 and resid 198 and name N)	(segid 3A4 and resid 248 and name CB)	7.43	0.14	0.15
	assign	(segid 3A4 and resid 198 and name O)	(segid 3A4 and resid 198 and name CB)	3.31	0.04	0.05
	assign	(segid 3A4 and resid 198 and name O)	(segid 3A4 and resid 198 and name CG)	4.57	0.06	0.05
	assign	(segid 3A4 and resid 198 and name O)	(segid 3A4 and resid 199 and name C)	2.91	0.08	0.07
25	assign	(segid 3A4 and resid 198 and name O)	(segid 3A4 and resid 199 and name CA)	2.79	0.02	0.02
	assign	(segid 3A4 and resid 198 and name O)	(segid 3A4 and resid 199 and name CB)	4.28	0.02	0.02
	assign	(segid 3A4 and resid 198 and name O)	(segid 3A4 and resid 199 and name N)	2.26	0.02	0.01
	assign	(segid 3A4 and resid 198 and name O)	(segid 3A4 and resid 199 and name O)	3.41	0.13	0.12
	assign	(segid 3A4 and resid 198 and name O)	(segid 3A4 and resid 200 and name C)	3.90	0.14	0.13
30	assign	(segid 3A4 and resid 198 and name O)	(segid 3A4 and resid 200 and name CA)	4.18	0.16	0.16
	assign	(segid 3A4 and resid 198 and name O)	(segid 3A4 and resid 200 and name N)	3.26	0.16	0.15
	assign	(segid 3A4 and resid 198 and name O)	(segid 3A4 and resid 200 and name O)	4.85	0.14	0.13
	assign	(segid 3A4 and resid 198 and name O)	(segid 3A4 and resid 201 and name C)	3.70	0.09	0.09
	assign	(segid 3A4 and resid 198 and name O)	(segid 3A4 and resid 201 and name CA)	3.53	0.11	0.11
35	assign	(segid 3A4 and resid 198 and name O)	(segid 3A4 and resid 201 and name CB)	3.38	0.08	0.09
	assign	(segid 3A4 and resid 198 and name O)	(segid 3A4 and resid 201 and name N)	3.04	0.16	0.17
	assign	(segid 3A4 and resid 198 and name O)	(segid 3A4 and resid 201 and name O)	4.90	0.09	0.08
	assign	(segid 3A4 and resid 198 and name O)	(segid 3A4 and resid 202 and name C)	5.12	0.14	0.14
	assign	(segid 3A4 and resid 198 and name O)	(segid 3A4 and resid 202 and name CA)	3.96	0.12	0.13
40	assign	(segid 3A4 and resid 198 and name O)	(segid 3A4 and resid 202 and name CB)	3.78	0.16	0.16
	assign	(segid 3A4 and resid 198 and name O)	(segid 3A4 and resid 202 and name CG1)	5.24	0.15	0.16
	assign	(segid 3A4 and resid 198 and name O)	(segid 3A4 and resid 202 and name N)	2.97	0.10	0.10
	assign	(segid 3A4 and resid 198 and name O)	(segid 3A4 and resid 202 and name O)	6.26	0.14	0.14
	assign	(segid 3A4 and resid 198 and name O)	(segid 3A4 and resid 203 and name C)	7.27	0.11	0.10
45	assign	(segid 3A4 and resid 198 and name O)	(segid 3A4 and resid 203 and name CA)	6.45	0.15	0.15
	assign	(segid 3A4 and resid 198 and name O)	(segid 3A4 and resid 203 and name CB)	6.66	0.15	0.15
	assign	(segid 3A4 and resid 198 and name O)	(segid 3A4 and resid 203 and name N)	5.11	0.15	0.15
	assign	(segid 3A4 and resid 198 and name O)	(segid 3A4 and resid 204 and name CB)	7.70	0.25	0.26
	assign	(segid 3A4 and resid 198 and name O)	(segid 3A4 and resid 204 and name N)	6.89	0.10	0.09
50	assign	(segid 3A4 and resid 198 and name O)	(segid 3A4 and resid 205 and name CB)	7.64	0.20	0.19
	assign	(segid 3A4 and resid 198 and name O)	(segid 3A4 and resid 205 and name N)	7.63	0.10	0.11
	assign	(segid 3A4 and resid 198 and name O)	(segid 3A4 and resid 245 and name CA)	6.36	0.52	0.52
	assign	(segid 3A4 and resid 198 and name O)	(segid 3A4 and resid 245 and name CB)	6.21	0.55	0.55
	assign	(segid 3A4 and resid 198 and name O)	(segid 3A4 and resid 245 and name N)	7.04	0.46	0.46
55	assign	(segid 3A4 and resid 198 and name O)	(segid 3A4 and resid 248 and name CB)	6.67	0.32	0.33
	assign	(segid 3A4 and resid 199 and name C)	(segid 3A4 and resid 199 and name CB)	2.52	0.04	0.05
	assign	(segid 3A4 and resid 199 and name C)	(segid 3A4 and resid 199 and name O)	1.23	0.01	0.02
	assign	(segid 3A4 and resid 199 and name C)	(segid 3A4 and resid 200 and name C)	3.04	0.04	0.05
	assign	(segid 3A4 and resid 199 and name C)	(segid 3A4 and resid 200 and name CA)	2.44	0.02	0.01
60	assign	(segid 3A4 and resid 199 and name C)	(segid 3A4 and resid 200 and name N)	1.33	0.00	0.00
	assign	(segid 3A4 and resid 199 and name C)	(segid 3A4 and resid 200 and name O)	3.90	0.08	0.09
	assign	(segid 3A4 and resid 199 and name C)	(segid 3A4 and resid 201 and name C)	4.54	0.10	0.10
	assign	(segid 3A4 and resid 199 and name C)	(segid 3A4 and resid 201 and name CA)	4.46	0.10	0.10
	assign	(segid 3A4 and resid 199 and name C)	(segid 3A4 and resid 201 and name CB)	5.20	0.08	0.08
65	assign	(segid 3A4 and resid 199 and name C)	(segid 3A4 and resid 201 and name N)	3.29	0.12	0.11
	assign	(segid 3A4 and resid 199 and name C)	(segid 3A4 and resid 201 and name O)	5.61	0.09	0.10
	assign	(segid 3A4 and resid 199 and name C)	(segid 3A4 and resid 202 and name C)	4.96	0.10	0.10
	assign	(segid 3A4 and resid 199 and name C)	(segid 3A4 and resid 202 and name CA)	4.58	0.12	0.12
	assign	(segid 3A4 and resid 199 and name C)	(segid 3A4 and resid 202 and name CB)	4.35	0.13	0.13
70	assign	(segid 3A4 and resid 199 and name C)	(segid 3A4 and resid 202 and name CG1)	5.51	0.09	0.08
	assign	(segid 3A4 and resid 199 and name C)	(segid 3A4 and resid 202 and name N)	3.83	0.13	0.13
	assign	(segid 3A4 and resid 199 and name C)	(segid 3A4 and resid 202 and name O)	6.18	0.10	0.10
	assign	(segid 3A4 and resid 199 and name C)	(segid 3A4 and resid 203 and name C)	6.23	0.07	0.08
	assign	(segid 3A4 and resid 199 and name C)	(segid 3A4 and resid 203 and name CA)	5.14	0.08	0.09
75	assign	(segid 3A4 and resid 199 and name C)	(segid 3A4 and resid 203 and name CB)	4.74	0.12	0.11
	assign	(segid 3A4 and resid 199 and name C)	(segid 3A4 and resid 203 and name N)	4.24	0.10	0.09
	assign	(segid 3A4 and resid 199 and name C)	(segid 3A4 and resid 203 and name O)	7.40	0.08	0.08
	assign	(segid 3A4 and resid 199 and name C)	(segid 3A4 and resid 204 and name CA)	7.33	0.09	0.09
	assign	(segid 3A4 and resid 199 and name C)	(segid 3A4 and resid 204 and name CB)	7.34	0.17	0.16
80	assign	(segid 3A4 and resid 199 and name C)	(segid 3A4 and resid 204 and name N)	6.07	0.08	0.08
	assign	(segid 3A4 and resid 199 and name CA)	(segid 3A4 and resid 199 and name C)	1.52	0.01	0.01
	assign	(segid 3A4 and resid 199 and name CA)	(segid 3A4 and resid 199 and name CB)	1.53	0.01	0.02
	assign	(segid 3A4 and resid 199 and name CA)	(segid 3A4 and resid 199 and name O)	2.40	0.01	0.01

	assign (segid 3A4 and resid 199 and name CA) (segid 3A4 and resid 200 and name C)	4.42	0.05	0.04
	assign (segid 3A4 and resid 199 and name CA) (segid 3A4 and resid 200 and name CA)	3.80	0.01	0.02
	assign (segid 3A4 and resid 199 and name CA) (segid 3A4 and resid 200 and name N)	2.43	0.01	0.01
	assign (segid 3A4 and resid 199 and name CA) (segid 3A4 and resid 200 and name O)	5.35	0.09	0.09
5	assign (segid 3A4 and resid 199 and name CA) (segid 3A4 and resid 201 and name C)	5.46	0.14	0.15
	assign (segid 3A4 and resid 199 and name CA) (segid 3A4 and resid 201 and name CA)	5.42	0.11	0.10
	assign (segid 3A4 and resid 199 and name CA) (segid 3A4 and resid 201 and name CB)	5.81	0.10	0.09
	assign (segid 3A4 and resid 199 and name CA) (segid 3A4 and resid 201 and name N)	4.35	0.10	0.11
	assign (segid 3A4 and resid 199 and name CA) (segid 3A4 and resid 201 and name O)	6.60	0.15	0.14
10	assign (segid 3A4 and resid 199 and name CA) (segid 3A4 and resid 202 and name C)	5.80	0.17	0.16
	assign (segid 3A4 and resid 199 and name CA) (segid 3A4 and resid 202 and name CA)	5.15	0.20	0.21
	assign (segid 3A4 and resid 199 and name CA) (segid 3A4 and resid 202 and name CB)	4.51	0.24	0.24
	assign (segid 3A4 and resid 199 and name CA) (segid 3A4 and resid 202 and name CG1)	5.60	0.19	0.20
	assign (segid 3A4 and resid 199 and name CA) (segid 3A4 and resid 202 and name N)	4.54	0.18	0.19
	assign (segid 3A4 and resid 199 and name CA) (segid 3A4 and resid 202 and name O)	7.00	0.18	0.17
15	assign (segid 3A4 and resid 199 and name CA) (segid 3A4 and resid 203 and name C)	7.49	0.10	0.10
	assign (segid 3A4 and resid 199 and name CA) (segid 3A4 and resid 203 and name CA)	6.30	0.11	0.11
	assign (segid 3A4 and resid 199 and name CA) (segid 3A4 and resid 203 and name CB)	6.00	0.12	0.12
	assign (segid 3A4 and resid 199 and name CA) (segid 3A4 and resid 203 and name N)	5.29	0.13	0.13
	assign (segid 3A4 and resid 199 and name CA) (segid 3A4 and resid 204 and name CA)	8.70	0.11	0.10
20	assign (segid 3A4 and resid 199 and name CA) (segid 3A4 and resid 204 and name CB)	8.73	0.17	0.16
	assign (segid 3A4 and resid 199 and name CA) (segid 3A4 and resid 204 and name N)	7.42	0.10	0.09
	assign (segid 3A4 and resid 199 and name CA) (segid 3A4 and resid 205 and name CA)	9.83	0.22	0.23
	assign (segid 3A4 and resid 199 and name CA) (segid 3A4 and resid 205 and name CB)	9.37	0.30	0.31
	assign (segid 3A4 and resid 199 and name CA) (segid 3A4 and resid 206 and name CA)	10.78	0.16	0.15
25	assign (segid 3A4 and resid 199 and name CA) (segid 3A4 and resid 206 and name CB)	10.11	0.16	0.16
	assign (segid 3A4 and resid 199 and name CA) (segid 3A4 and resid 207 and name CA)	12.83	0.18	0.17
	assign (segid 3A4 and resid 199 and name CA) (segid 3A4 and resid 207 and name CB)	12.53	0.31	0.30
	assign (segid 3A4 and resid 199 and name CA) (segid 3A4 and resid 219 and name CA)	15.52	0.52	0.53
	assign (segid 3A4 and resid 199 and name CA) (segid 3A4 and resid 219 and name CB)	14.57	0.43	0.43
30	assign (segid 3A4 and resid 199 and name CA) (segid 3A4 and resid 220 and name CA)	14.28	0.78	0.77
	assign (segid 3A4 and resid 199 and name CA) (segid 3A4 and resid 220 and name CB)	14.29	0.92	0.92
	assign (segid 3A4 and resid 199 and name CA) (segid 3A4 and resid 221 and name CA)	10.83	0.70	0.69
	assign (segid 3A4 and resid 199 and name CA) (segid 3A4 and resid 221 and name CB)	9.79	0.65	0.64
	assign (segid 3A4 and resid 199 and name CA) (segid 3A4 and resid 222 and name CA)	12.82	0.68	0.68
35	assign (segid 3A4 and resid 199 and name CA) (segid 3A4 and resid 222 and name CB)	13.84	0.67	0.67
	assign (segid 3A4 and resid 199 and name CA) (segid 3A4 and resid 223 and name CA)	15.28	0.73	0.74
	assign (segid 3A4 and resid 199 and name CA) (segid 3A4 and resid 223 and name CB)	16.12	0.77	0.76
	assign (segid 3A4 and resid 199 and name CA) (segid 3A4 and resid 224 and name CA)	13.14	0.78	0.78
	assign (segid 3A4 and resid 199 and name CA) (segid 3A4 and resid 224 and name CB)	12.20	0.75	0.74
40	assign (segid 3A4 and resid 199 and name CA) (segid 3A4 and resid 225 and name CA)	11.63	1.11	1.10
	assign (segid 3A4 and resid 199 and name CA) (segid 3A4 and resid 225 and name CB)	10.96	1.10	1.11
	assign (segid 3A4 and resid 199 and name CA) (segid 3A4 and resid 226 and name CA)	15.20	1.20	1.21
	assign (segid 3A4 and resid 199 and name CA) (segid 3A4 and resid 240 and name CA)	11.95	0.58	0.57
	assign (segid 3A4 and resid 199 and name CA) (segid 3A4 and resid 240 and name CB)	12.49	0.55	0.56
45	assign (segid 3A4 and resid 199 and name CA) (segid 3A4 and resid 241 and name CA)	8.28	0.59	0.59
	assign (segid 3A4 and resid 199 and name CA) (segid 3A4 and resid 241 and name CB)	7.83	0.70	0.70
	assign (segid 3A4 and resid 199 and name CA) (segid 3A4 and resid 242 and name CA)	8.75	0.73	0.73
	assign (segid 3A4 and resid 199 and name CA) (segid 3A4 and resid 242 and name CB)	9.82	0.81	0.82
50	assign (segid 3A4 and resid 199 and name CA) (segid 3A4 and resid 243 and name CA)	10.99	0.48	0.49
	assign (segid 3A4 and resid 199 and name CA) (segid 3A4 and resid 243 and name CB)	12.24	0.46	0.46
	assign (segid 3A4 and resid 199 and name CA) (segid 3A4 and resid 244 and name CA)	9.08	0.37	0.36
	assign (segid 3A4 and resid 199 and name CA) (segid 3A4 and resid 244 and name CB)	8.56	0.53	0.53
	assign (segid 3A4 and resid 199 and name CA) (segid 3A4 and resid 245 and name CA)	6.62	0.34	0.34
	assign (segid 3A4 and resid 199 and name CA) (segid 3A4 and resid 245 and name CB)	5.86	0.44	0.43
55	assign (segid 3A4 and resid 199 and name CA) (segid 3A4 and resid 245 and name N)	7.29	0.32	0.32
	assign (segid 3A4 and resid 199 and name CA) (segid 3A4 and resid 246 and name CA)	9.97	0.50	0.50
	assign (segid 3A4 and resid 199 and name CA) (segid 3A4 and resid 246 and name CB)	10.95	0.51	0.50
	assign (segid 3A4 and resid 199 and name CA) (segid 3A4 and resid 247 and name CA)	11.71	0.15	0.14
	assign (segid 3A4 and resid 199 and name CA) (segid 3A4 and resid 247 and name CB)	12.07	0.17	0.17
60	assign (segid 3A4 and resid 199 and name CA) (segid 3A4 and resid 248 and name CA)	9.80	0.22	0.22
	assign (segid 3A4 and resid 199 and name CA) (segid 3A4 and resid 248 and name CB)	8.48	0.21	0.21
	assign (segid 3A4 and resid 199 and name CA) (segid 3A4 and resid 249 and name CA)	10.35	0.75	0.74
	assign (segid 3A4 and resid 199 and name CA) (segid 3A4 and resid 250 and name CA)	13.81	0.60	0.61
	assign (segid 3A4 and resid 199 and name CA) (segid 3A4 and resid 250 and name CB)	14.34	0.48	0.49
65	assign (segid 3A4 and resid 199 and name CA) (segid 3A4 and resid 251 and name CA)	14.59	0.49	0.50
	assign (segid 3A4 and resid 199 and name CA) (segid 3A4 and resid 251 and name CB)	14.11	0.40	0.40
	assign (segid 3A4 and resid 199 and name CA) (segid 3A4 and resid 252 and name CA)	13.89	0.76	0.76
	assign (segid 3A4 and resid 199 and name CA) (segid 3A4 and resid 252 and name CB)	12.63	0.82	0.82
	assign (segid 3A4 and resid 199 and name CA) (segid 3A4 and resid 253 and name CA)	15.88	0.81	0.81
70	assign (segid 3A4 and resid 199 and name CA) (segid 3A4 and resid 254 and name CA)	18.51	0.66	0.66
	assign (segid 3A4 and resid 199 and name CB) (segid 3A4 and resid 200 and name C)	5.48	0.07	0.06
	assign (segid 3A4 and resid 199 and name CB) (segid 3A4 and resid 200 and name CA)	4.52	0.04	0.05
	assign (segid 3A4 and resid 199 and name CB) (segid 3A4 and resid 200 and name N)	3.20	0.06	0.06
	assign (segid 3A4 and resid 199 and name CB) (segid 3A4 and resid 200 and name O)	6.37	0.10	0.10
75	assign (segid 3A4 and resid 199 and name CB) (segid 3A4 and resid 201 and name C)	6.89	0.15	0.16
	assign (segid 3A4 and resid 199 and name CB) (segid 3A4 and resid 201 and name CA)	6.80	0.10	0.11
	assign (segid 3A4 and resid 199 and name CB) (segid 3A4 and resid 201 and name CB)	7.25	0.10	0.10
	assign (segid 3A4 and resid 199 and name CB) (segid 3A4 and resid 201 and name N)	5.63	0.10	0.10
	assign (segid 3A4 and resid 199 and name CB) (segid 3A4 and resid 202 and name C)	6.96	0.22	0.23
80	assign (segid 3A4 and resid 199 and name CB) (segid 3A4 and resid 202 and name CA)	6.49	0.26	0.26
	assign (segid 3A4 and resid 199 and name CB) (segid 3A4 and resid 202 and name CB)	5.73	0.32	0.33
	assign (segid 3A4 and resid 199 and name CB) (segid 3A4 and resid 202 and name CG1)	6.61	0.29	0.30

	assign (segid 3A4 and resid 199 and name O) (segid 3A4 and resid 200 and name N)	2.24	0.01	0.02
	assign (segid 3A4 and resid 199 and name O) (segid 3A4 and resid 200 and name O)	3.52	0.11	0.11
	assign (segid 3A4 and resid 199 and name O) (segid 3A4 and resid 201 and name C)	4.12	0.13	0.12
	assign (segid 3A4 and resid 199 and name O) (segid 3A4 and resid 201 and name CA)	4.41	0.13	0.12
5	assign (segid 3A4 and resid 199 and name O) (segid 3A4 and resid 201 and name CB)	5.36	0.06	0.07
	assign (segid 3A4 and resid 199 and name O) (segid 3A4 and resid 201 and name N)	3.46	0.13	0.13
	assign (segid 3A4 and resid 199 and name O) (segid 3A4 and resid 201 and name O)	5.04	0.10	0.10
	assign (segid 3A4 and resid 199 and name O) (segid 3A4 and resid 202 and name C)	3.93	0.09	0.09
	assign (segid 3A4 and resid 199 and name O) (segid 3A4 and resid 202 and name CA)	3.81	0.09	0.10
	assign (segid 3A4 and resid 199 and name O) (segid 3A4 and resid 202 and name CB)	3.66	0.09	0.10
10	assign (segid 3A4 and resid 199 and name O) (segid 3A4 and resid 202 and name CG1)	4.67	0.06	0.07
	assign (segid 3A4 and resid 199 and name O) (segid 3A4 and resid 202 and name N)	3.34	0.13	0.13
	assign (segid 3A4 and resid 199 and name O) (segid 3A4 and resid 202 and name O)	5.11	0.09	0.10
	assign (segid 3A4 and resid 199 and name O) (segid 3A4 and resid 203 and name C)	5.15	0.09	0.09
	assign (segid 3A4 and resid 199 and name O) (segid 3A4 and resid 203 and name CA)	3.97	0.09	0.10
15	assign (segid 3A4 and resid 199 and name O) (segid 3A4 and resid 203 and name CB)	3.66	0.11	0.12
	assign (segid 3A4 and resid 199 and name O) (segid 3A4 and resid 203 and name N)	3.10	0.10	0.10
	assign (segid 3A4 and resid 199 and name O) (segid 3A4 and resid 203 and name O)	6.28	0.09	0.10
	assign (segid 3A4 and resid 199 and name O) (segid 3A4 and resid 204 and name C)	7.32	0.12	0.12
	assign (segid 3A4 and resid 199 and name O) (segid 3A4 and resid 204 and name CA)	6.49	0.12	0.13
20	assign (segid 3A4 and resid 199 and name O) (segid 3A4 and resid 204 and name CB)	6.71	0.19	0.20
	assign (segid 3A4 and resid 199 and name O) (segid 3A4 and resid 204 and name N)	5.15	0.11	0.10
	assign (segid 3A4 and resid 199 and name O) (segid 3A4 and resid 205 and name N)	6.90	0.15	0.15
	assign (segid 3A4 and resid 199 and name O) (segid 3A4 and resid 19 and name CB)	2.52	0.01	0.02
	assign (segid 3A4 and resid 19 and name C) (segid 3A4 and resid 19 and name O)	1.22	0.01	0.02
25	assign (segid 3A4 and resid 19 and name C) (segid 3A4 and resid 20 and name C)	3.50	0.05	0.05
	assign (segid 3A4 and resid 19 and name C) (segid 3A4 and resid 20 and name CA)	2.44	0.01	0.01
	assign (segid 3A4 and resid 19 and name C) (segid 3A4 and resid 20 and name CB)	3.39	0.09	0.09
	assign (segid 3A4 and resid 19 and name C) (segid 3A4 and resid 20 and name N)	1.33	0.00	0.00
	assign (segid 3A4 and resid 19 and name C) (segid 3A4 and resid 20 and name O)	4.10	0.06	0.06
30	assign (segid 3A4 and resid 19 and name C) (segid 3A4 and resid 21 and name C)	6.56	0.14	0.14
	assign (segid 3A4 and resid 19 and name C) (segid 3A4 and resid 21 and name CA)	5.46	0.14	0.15
	assign (segid 3A4 and resid 19 and name C) (segid 3A4 and resid 21 and name CB)	5.66	0.19	0.19
	assign (segid 3A4 and resid 19 and name C) (segid 3A4 and resid 21 and name N)	4.21	0.15	0.15
	assign (segid 3A4 and resid 19 and name C) (segid 3A4 and resid 21 and name O)	6.50	0.15	0.16
35	assign (segid 3A4 and resid 19 and name C) (segid 3A4 and resid 22 and name N)	7.75	0.12	0.11
	assign (segid 3A4 and resid 19 and name C) (segid 3A4 and resid 32 and name C)	5.27	0.17	0.17
	assign (segid 3A4 and resid 19 and name C) (segid 3A4 and resid 32 and name CA)	6.60	0.15	0.15
	assign (segid 3A4 and resid 19 and name C) (segid 3A4 and resid 32 and name CB)	6.88	0.16	0.16
	assign (segid 3A4 and resid 19 and name C) (segid 3A4 and resid 32 and name N)	6.90	0.13	0.14
40	assign (segid 3A4 and resid 19 and name C) (segid 3A4 and resid 32 and name O)	4.26	0.16	0.16
	assign (segid 3A4 and resid 19 and name C) (segid 3A4 and resid 33 and name C)	4.97	0.34	0.35
	assign (segid 3A4 and resid 19 and name C) (segid 3A4 and resid 33 and name CA)	4.79	0.34	0.34
	assign (segid 3A4 and resid 19 and name C) (segid 3A4 and resid 33 and name CB)	5.75	0.42	0.43
	assign (segid 3A4 and resid 19 and name C) (segid 3A4 and resid 33 and name N)	5.55	0.25	0.24
45	assign (segid 3A4 and resid 19 and name C) (segid 3A4 and resid 33 and name O)	6.15	0.36	0.35
	assign (segid 3A4 and resid 19 and name C) (segid 3A4 and resid 34 and name C)	5.34	0.26	0.26
	assign (segid 3A4 and resid 19 and name C) (segid 3A4 and resid 34 and name CA)	4.85	0.26	0.26
	assign (segid 3A4 and resid 19 and name C) (segid 3A4 and resid 34 and name CB)	4.54	0.25	0.25
	assign (segid 3A4 and resid 19 and name C) (segid 3A4 and resid 34 and name N)	4.13	0.30	0.30
50	assign (segid 3A4 and resid 19 and name C) (segid 3A4 and resid 34 and name O)	6.41	0.22	0.23
	assign (segid 3A4 and resid 19 and name C) (segid 3A4 and resid 35 and name C)	7.03	0.39	0.39
	assign (segid 3A4 and resid 19 and name C) (segid 3A4 and resid 35 and name CA)	5.91	0.36	0.35
	assign (segid 3A4 and resid 19 and name C) (segid 3A4 and resid 35 and name N)	4.95	0.36	0.36
	assign (segid 3A4 and resid 19 and name C) (segid 3A4 and resid 35 and name O)	7.01	0.43	0.42
55	assign (segid 3A4 and resid 19 and name C) (segid 3A4 and resid 38 and name CB)	5.83	0.67	0.67
	assign (segid 3A4 and resid 19 and name C) (segid 3A4 and resid 19 and name C)	1.53	0.00	0.00
	assign (segid 3A4 and resid 19 and name CA) (segid 3A4 and resid 19 and name CB)	1.52	0.01	0.01
	assign (segid 3A4 and resid 19 and name CA) (segid 3A4 and resid 19 and name O)	2.38	0.01	0.02
	assign (segid 3A4 and resid 19 and name CA) (segid 3A4 and resid 20 and name C)	4.68	0.05	0.05
60	assign (segid 3A4 and resid 19 and name CA) (segid 3A4 and resid 20 and name CA)	3.82	0.01	0.02
	assign (segid 3A4 and resid 19 and name CA) (segid 3A4 and resid 20 and name CB)	4.67	0.07	0.07
	assign (segid 3A4 and resid 19 and name CA) (segid 3A4 and resid 20 and name N)	2.45	0.03	0.02
	assign (segid 3A4 and resid 19 and name CA) (segid 3A4 and resid 20 and name O)	5.02	0.10	0.09
	assign (segid 3A4 and resid 19 and name CA) (segid 3A4 and resid 21 and name CA)	6.52	0.16	0.16
65	assign (segid 3A4 and resid 19 and name CA) (segid 3A4 and resid 21 and name CB)	6.46	0.22	0.23
	assign (segid 3A4 and resid 19 and name CA) (segid 3A4 and resid 21 and name N)	5.42	0.15	0.16
	assign (segid 3A4 and resid 19 and name CA) (segid 3A4 and resid 22 and name CA)	10.13	0.16	0.16
	assign (segid 3A4 and resid 19 and name CA) (segid 3A4 and resid 23 and name CA)	12.38	0.31	0.31
	assign (segid 3A4 and resid 19 and name CA) (segid 3A4 and resid 23 and name CB)	12.14	0.39	0.40
70	assign (segid 3A4 and resid 19 and name CA) (segid 3A4 and resid 24 and name CA)	16.08	0.29	0.28
	assign (segid 3A4 and resid 19 and name CA) (segid 3A4 and resid 24 and name CB)	16.80	0.28	0.28
	assign (segid 3A4 and resid 19 and name CA) (segid 3A4 and resid 25 and name CA)	18.12	0.57	0.58
	assign (segid 3A4 and resid 19 and name CA) (segid 3A4 and resid 29 and name CA)	16.20	0.23	0.23
	assign (segid 3A4 and resid 19 and name CA) (segid 3A4 and resid 30 and name CA)	13.54	0.21	0.21
75	assign (segid 3A4 and resid 19 and name CA) (segid 3A4 and resid 317 and name CA)	18.76	0.38	0.38
	assign (segid 3A4 and resid 19 and name CA) (segid 3A4 and resid 31 and name CA)	9.99	0.16	0.17
	assign (segid 3A4 and resid 19 and name CA) (segid 3A4 and resid 31 and name CB)	9.88	0.12	0.13
	assign (segid 3A4 and resid 19 and name CA) (segid 3A4 and resid 322 and name CA)	16.22	0.52	0.51
	assign (segid 3A4 and resid 19 and name CA) (segid 3A4 and resid 323 and name CA)	16.60	0.34	0.33
80	assign (segid 3A4 and resid 19 and name CA) (segid 3A4 and resid 323 and name CB)	15.80	0.46	0.45
	assign (segid 3A4 and resid 19 and name CA) (segid 3A4 and resid 324 and name CA)	17.89	0.30	0.30
	assign (segid 3A4 and resid 19 and name CA) (segid 3A4 and resid 324 and name CB)	19.30	0.34	0.33

	assign	(segid 3A4 and resid 19 and name CA)	(segid 3A4 and resid 325 and name CA)	17.64	0.24	0.23
	assign	(segid 3A4 and resid 19 and name CA)	(segid 3A4 and resid 325 and name CB)	16.83	0.31	0.30
	assign	(segid 3A4 and resid 19 and name CA)	(segid 3A4 and resid 329 and name CA)	16.20	0.84	0.84
	assign	(segid 3A4 and resid 19 and name CA)	(segid 3A4 and resid 329 and name CB)	15.88	0.83	0.82
5	assign	(segid 3A4 and resid 19 and name CA)	(segid 3A4 and resid 32 and name C)	6.62	0.21	0.20
	assign	(segid 3A4 and resid 19 and name CA)	(segid 3A4 and resid 32 and name CA)	7.92	0.19	0.20
	assign	(segid 3A4 and resid 19 and name CA)	(segid 3A4 and resid 32 and name CB)	8.04	0.21	0.21
	assign	(segid 3A4 and resid 19 and name CA)	(segid 3A4 and resid 32 and name O)	5.63	0.19	0.18
	assign	(segid 3A4 and resid 19 and name CA)	(segid 3A4 and resid 330 and name CA)	13.82	0.90	0.90
	assign	(segid 3A4 and resid 19 and name CA)	(segid 3A4 and resid 330 and name CB)	14.57	0.96	0.96
10	assign	(segid 3A4 and resid 19 and name CA)	(segid 3A4 and resid 331 and name CA)	10.59	0.87	0.86
	assign	(segid 3A4 and resid 19 and name CA)	(segid 3A4 and resid 331 and name CB)	10.02	0.74	0.75
	assign	(segid 3A4 and resid 19 and name CA)	(segid 3A4 and resid 332 and name CA)	9.04	1.21	1.22
	assign	(segid 3A4 and resid 19 and name CA)	(segid 3A4 and resid 333 and name CA)	11.07	1.41	1.42
15	assign	(segid 3A4 and resid 19 and name CA)	(segid 3A4 and resid 335 and name CA)	10.41	0.90	0.91
	assign	(segid 3A4 and resid 19 and name CA)	(segid 3A4 and resid 336 and name CA)	13.57	0.76	0.76
	assign	(segid 3A4 and resid 19 and name CA)	(segid 3A4 and resid 336 and name CB)	14.76	0.73	0.72
	assign	(segid 3A4 and resid 19 and name CA)	(segid 3A4 and resid 337 and name CA)	13.95	0.82	0.82
	assign	(segid 3A4 and resid 19 and name CA)	(segid 3A4 and resid 337 and name CB)	13.32	0.75	0.75
20	assign	(segid 3A4 and resid 19 and name CA)	(segid 3A4 and resid 338 and name CA)	17.54	0.78	0.78
	assign	(segid 3A4 and resid 19 and name CA)	(segid 3A4 and resid 338 and name CB)	18.13	0.87	0.87
	assign	(segid 3A4 and resid 19 and name CA)	(segid 3A4 and resid 33 and name C)	5.88	0.41	0.41
	assign	(segid 3A4 and resid 19 and name CA)	(segid 3A4 and resid 33 and name CA)	6.00	0.37	0.36
	assign	(segid 3A4 and resid 19 and name CA)	(segid 3A4 and resid 33 and name CB)	6.92	0.45	0.45
25	assign	(segid 3A4 and resid 19 and name CA)	(segid 3A4 and resid 33 and name N)	6.83	0.28	0.28
	assign	(segid 3A4 and resid 19 and name CA)	(segid 3A4 and resid 33 and name O)	6.98	0.42	0.43
	assign	(segid 3A4 and resid 19 and name CA)	(segid 3A4 and resid 341 and name CA)	16.80	0.20	0.20
	assign	(segid 3A4 and resid 19 and name CA)	(segid 3A4 and resid 341 and name CB)	15.71	0.30	0.29
	assign	(segid 3A4 and resid 19 and name CA)	(segid 3A4 and resid 342 and name CA)	15.71	0.17	0.17
30	assign	(segid 3A4 and resid 19 and name CA)	(segid 3A4 and resid 343 and name CA)	12.53	0.24	0.24
	assign	(segid 3A4 and resid 19 and name CA)	(segid 3A4 and resid 343 and name CB)	12.19	0.31	0.30
	assign	(segid 3A4 and resid 19 and name CA)	(segid 3A4 and resid 344 and name CA)	12.00	0.27	0.28
	assign	(segid 3A4 and resid 19 and name CA)	(segid 3A4 and resid 344 and name CB)	12.15	0.24	0.24
	assign	(segid 3A4 and resid 19 and name CA)	(segid 3A4 and resid 345 and name CA)	10.81	0.56	0.56
35	assign	(segid 3A4 and resid 19 and name CA)	(segid 3A4 and resid 345 and name CB)	11.55	0.65	0.64
	assign	(segid 3A4 and resid 19 and name CA)	(segid 3A4 and resid 346 and name CA)	10.70	0.79	0.80
	assign	(segid 3A4 and resid 19 and name CA)	(segid 3A4 and resid 346 and name CB)	9.84	0.85	0.84
	assign	(segid 3A4 and resid 19 and name CA)	(segid 3A4 and resid 347 and name CA)	12.96	0.79	0.80
	assign	(segid 3A4 and resid 19 and name CA)	(segid 3A4 and resid 347 and name CB)	14.42	0.80	0.79
40	assign	(segid 3A4 and resid 19 and name CA)	(segid 3A4 and resid 348 and name CA)	13.53	0.66	0.67
	assign	(segid 3A4 and resid 19 and name CA)	(segid 3A4 and resid 349 and name CA)	10.11	0.68	0.69
	assign	(segid 3A4 and resid 19 and name CA)	(segid 3A4 and resid 349 and name CB)	8.85	0.66	0.67
	assign	(segid 3A4 and resid 19 and name CA)	(segid 3A4 and resid 34 and name C)	5.32	0.42	0.42
	assign	(segid 3A4 and resid 19 and name CA)	(segid 3A4 and resid 34 and name CA)	5.13	0.38	0.39
45	assign	(segid 3A4 and resid 19 and name CA)	(segid 3A4 and resid 34 and name CB)	4.60	0.35	0.36
	assign	(segid 3A4 and resid 19 and name CA)	(segid 3A4 and resid 34 and name N)	4.81	0.40	0.39
	assign	(segid 3A4 and resid 19 and name CA)	(segid 3A4 and resid 34 and name O)	6.23	0.36	0.36
	assign	(segid 3A4 and resid 19 and name CA)	(segid 3A4 and resid 350 and name CA)	10.50	0.85	0.86
	assign	(segid 3A4 and resid 19 and name CA)	(segid 3A4 and resid 350 and name CB)	11.01	0.92	0.91
50	assign	(segid 3A4 and resid 19 and name CA)	(segid 3A4 and resid 351 and name CA)	13.89	0.79	0.79
	assign	(segid 3A4 and resid 19 and name CA)	(segid 3A4 and resid 352 and name CA)	13.02	0.89	0.89
	assign	(segid 3A4 and resid 19 and name CA)	(segid 3A4 and resid 352 and name CB)	13.03	0.94	0.94
	assign	(segid 3A4 and resid 19 and name CA)	(segid 3A4 and resid 353 and name CA)	10.74	0.91	0.90
	assign	(segid 3A4 and resid 19 and name CA)	(segid 3A4 and resid 353 and name CB)	10.18	0.94	0.93
55	assign	(segid 3A4 and resid 19 and name CA)	(segid 3A4 and resid 354 and name CA)	12.87	0.91	0.90
	assign	(segid 3A4 and resid 19 and name CA)	(segid 3A4 and resid 354 and name CB)	12.83	0.93	0.92
	assign	(segid 3A4 and resid 19 and name CA)	(segid 3A4 and resid 355 and name CA)	12.73	1.15	1.15
	assign	(segid 3A4 and resid 19 and name CA)	(segid 3A4 and resid 355 and name CB)	11.70	1.23	1.24
	assign	(segid 3A4 and resid 19 and name CA)	(segid 3A4 and resid 356 and name CA)	14.42	0.88	0.87
60	assign	(segid 3A4 and resid 19 and name CA)	(segid 3A4 and resid 356 and name CB)	13.82	0.81	0.81
	assign	(segid 3A4 and resid 19 and name CA)	(segid 3A4 and resid 357 and name CA)	16.50	0.87	0.88
	assign	(segid 3A4 and resid 19 and name CA)	(segid 3A4 and resid 357 and name CB)	16.46	0.94	0.93
	assign	(segid 3A4 and resid 19 and name CA)	(segid 3A4 and resid 35 and name C)	6.89	0.56	0.55
	assign	(segid 3A4 and resid 19 and name CA)	(segid 3A4 and resid 35 and name CA)	5.59	0.54	0.53
	assign	(segid 3A4 and resid 19 and name CA)	(segid 3A4 and resid 35 and name N)	4.88	0.55	0.55
65	assign	(segid 3A4 and resid 19 and name CA)	(segid 3A4 and resid 360 and name CA)	16.93	0.69	0.69
	assign	(segid 3A4 and resid 19 and name CA)	(segid 3A4 and resid 360 and name CB)	15.42	0.68	0.69
	assign	(segid 3A4 and resid 19 and name CA)	(segid 3A4 and resid 36 and name CA)	9.24	0.57	0.57
	assign	(segid 3A4 and resid 19 and name CA)	(segid 3A4 and resid 37 and name CA)	9.42	0.62	0.63
70	assign	(segid 3A4 and resid 19 and name CA)	(segid 3A4 and resid 37 and name CB)	9.14	0.62	0.61
	assign	(segid 3A4 and resid 19 and name CA)	(segid 3A4 and resid 381 and name CA)	17.38	0.69	0.69
	assign	(segid 3A4 and resid 19 and name CA)	(segid 3A4 and resid 382 and name CA)	16.57	0.42	0.42
	assign	(segid 3A4 and resid 19 and name CA)	(segid 3A4 and resid 382 and name CB)	15.24	0.41	0.42
	assign	(segid 3A4 and resid 19 and name CA)	(segid 3A4 and resid 383 and name CA)	18.71	0.37	0.37
75	assign	(segid 3A4 and resid 19 and name CA)	(segid 3A4 and resid 385 and name CA)	18.36	0.46	0.45
	assign	(segid 3A4 and resid 19 and name CA)	(segid 3A4 and resid 386 and name CA)	18.35	0.42	0.43
	assign	(segid 3A4 and resid 19 and name CA)	(segid 3A4 and resid 38 and name CA)	7.73	0.79	0.80
	assign	(segid 3A4 and resid 19 and name CA)	(segid 3A4 and resid 38 and name CB)	6.36	0.83	0.82
	assign	(segid 3A4 and resid 19 and name CA)	(segid 3A4 and resid 39 and name CA)	9.76	0.75	0.75
	assign	(segid 3A4 and resid 19 and name CA)	(segid 3A4 and resid 39 and name CB)	9.84	0.76	0.77
80	assign	(segid 3A4 and resid 19 and name CA)	(segid 3A4 and resid 40 and name CA)	12.79	0.70	0.71
	assign	(segid 3A4 and resid 19 and name CA)	(segid 3A4 and resid 40 and name CB)	13.17	0.68	0.69
	assign	(segid 3A4 and resid 19 and name CA)	(segid 3A4 and resid 41 and name CA)	12.67	0.70	0.70

	assign	(segid 3A4 and resid 19 and name CA)	(segid 3A4 and resid 41 and name CB)	11.75	0.71	0.71
	assign	(segid 3A4 and resid 19 and name CA)	(segid 3A4 and resid 42 and name CA)	12.61	0.73	0.72
	assign	(segid 3A4 and resid 19 and name CA)	(segid 3A4 and resid 42 and name CB)	11.59	0.70	0.71
5	assign	(segid 3A4 and resid 19 and name CB)	(segid 3A4 and resid 20 and name C)	5.63	0.10	0.09
	assign	(segid 3A4 and resid 19 and name CB)	(segid 3A4 and resid 20 and name CA)	4.60	0.07	0.06
	assign	(segid 3A4 and resid 19 and name CB)	(segid 3A4 and resid 20 and name CB)	5.01	0.08	0.07
	assign	(segid 3A4 and resid 19 and name CB)	(segid 3A4 and resid 20 and name N)	3.28	0.09	0.10
	assign	(segid 3A4 and resid 19 and name CB)	(segid 3A4 and resid 20 and name O)	5.84	0.08	0.09
10	assign	(segid 3A4 and resid 19 and name CB)	(segid 3A4 and resid 21 and name CA)	7.70	0.18	0.17
	assign	(segid 3A4 and resid 19 and name CB)	(segid 3A4 and resid 21 and name CB)	7.79	0.26	0.26
	assign	(segid 3A4 and resid 19 and name CB)	(segid 3A4 and resid 21 and name N)	6.55	0.17	0.16
	assign	(segid 3A4 and resid 19 and name CB)	(segid 3A4 and resid 22 and name CA)	11.30	0.13	0.13
	assign	(segid 3A4 and resid 19 and name CB)	(segid 3A4 and resid 23 and name CA)	13.74	0.30	0.29
	assign	(segid 3A4 and resid 19 and name CB)	(segid 3A4 and resid 23 and name CB)	13.54	0.38	0.38
15	assign	(segid 3A4 and resid 19 and name CB)	(segid 3A4 and resid 24 and name CA)	17.41	0.26	0.26
	assign	(segid 3A4 and resid 19 and name CB)	(segid 3A4 and resid 24 and name CB)	18.12	0.28	0.29
	assign	(segid 3A4 and resid 19 and name CB)	(segid 3A4 and resid 29 and name CA)	17.32	0.21	0.21
	assign	(segid 3A4 and resid 19 and name CB)	(segid 3A4 and resid 30 and name CA)	14.58	0.18	0.17
20	assign	(segid 3A4 and resid 19 and name CB)	(segid 3A4 and resid 317 and name CA)	19.20	0.41	0.41
	assign	(segid 3A4 and resid 19 and name CB)	(segid 3A4 and resid 31 and name CA)	10.93	0.13	0.14
	assign	(segid 3A4 and resid 19 and name CB)	(segid 3A4 and resid 31 and name CB)	10.65	0.09	0.09
	assign	(segid 3A4 and resid 19 and name CB)	(segid 3A4 and resid 322 and name CA)	16.81	0.59	0.60
	assign	(segid 3A4 and resid 19 and name CB)	(segid 3A4 and resid 323 and name CA)	16.99	0.39	0.38
25	assign	(segid 3A4 and resid 19 and name CB)	(segid 3A4 and resid 323 and name CB)	16.08	0.48	0.48
	assign	(segid 3A4 and resid 19 and name CB)	(segid 3A4 and resid 324 and name CA)	18.28	0.36	0.35
	assign	(segid 3A4 and resid 19 and name CB)	(segid 3A4 and resid 325 and name CA)	17.80	0.26	0.26
	assign	(segid 3A4 and resid 19 and name CB)	(segid 3A4 and resid 325 and name CB)	16.99	0.30	0.29
	assign	(segid 3A4 and resid 19 and name CB)	(segid 3A4 and resid 329 and name CA)	15.89	0.83	0.82
30	assign	(segid 3A4 and resid 19 and name CB)	(segid 3A4 and resid 329 and name CB)	15.57	0.79	0.80
	assign	(segid 3A4 and resid 19 and name CB)	(segid 3A4 and resid 32 and name C)	7.59	0.19	0.19
	assign	(segid 3A4 and resid 19 and name CB)	(segid 3A4 and resid 32 and name CA)	8.99	0.17	0.17
	assign	(segid 3A4 and resid 19 and name CB)	(segid 3A4 and resid 32 and name CB)	9.27	0.19	0.19
	assign	(segid 3A4 and resid 19 and name CB)	(segid 3A4 and resid 32 and name O)	6.68	0.17	0.17
35	assign	(segid 3A4 and resid 19 and name CB)	(segid 3A4 and resid 330 and name CA)	13.33	0.92	0.92
	assign	(segid 3A4 and resid 19 and name CB)	(segid 3A4 and resid 330 and name CB)	14.00	1.00	0.99
	assign	(segid 3A4 and resid 19 and name CB)	(segid 3A4 and resid 331 and name CA)	9.99	0.89	0.88
	assign	(segid 3A4 and resid 19 and name CB)	(segid 3A4 and resid 331 and name CB)	9.58	0.75	0.75
	assign	(segid 3A4 and resid 19 and name CB)	(segid 3A4 and resid 332 and name CA)	8.08	1.25	1.25
40	assign	(segid 3A4 and resid 19 and name CB)	(segid 3A4 and resid 333 and name CA)	10.35	1.39	1.38
	assign	(segid 3A4 and resid 19 and name CB)	(segid 3A4 and resid 335 and name CA)	10.22	0.91	0.92
	assign	(segid 3A4 and resid 19 and name CB)	(segid 3A4 and resid 336 and name CA)	13.47	0.77	0.77
	assign	(segid 3A4 and resid 19 and name CB)	(segid 3A4 and resid 336 and name CB)	14.66	0.76	0.75
	assign	(segid 3A4 and resid 19 and name CB)	(segid 3A4 and resid 337 and name CA)	14.09	0.79	0.79
45	assign	(segid 3A4 and resid 19 and name CB)	(segid 3A4 and resid 337 and name CB)	13.44	0.71	0.72
	assign	(segid 3A4 and resid 19 and name CB)	(segid 3A4 and resid 338 and name CA)	17.78	0.76	0.76
	assign	(segid 3A4 and resid 19 and name CB)	(segid 3A4 and resid 338 and name CB)	18.45	0.83	0.83
	assign	(segid 3A4 and resid 19 and name CB)	(segid 3A4 and resid 33 and name C)	6.50	0.44	0.44
	assign	(segid 3A4 and resid 19 and name CB)	(segid 3A4 and resid 33 and name CA)	6.59	0.39	0.38
	assign	(segid 3A4 and resid 19 and name CB)	(segid 3A4 and resid 33 and name CB)	7.23	0.51	0.51
50	assign	(segid 3A4 and resid 19 and name CB)	(segid 3A4 and resid 341 and name CA)	17.37	0.20	0.19
	assign	(segid 3A4 and resid 19 and name CB)	(segid 3A4 and resid 341 and name CB)	16.24	0.28	0.27
	assign	(segid 3A4 and resid 19 and name CB)	(segid 3A4 and resid 342 and name CA)	16.41	0.21	0.22
	assign	(segid 3A4 and resid 19 and name CB)	(segid 3A4 and resid 343 and name CA)	13.16	0.29	0.29
	assign	(segid 3A4 and resid 19 and name CB)	(segid 3A4 and resid 343 and name CB)	12.66	0.37	0.36
55	assign	(segid 3A4 and resid 19 and name CB)	(segid 3A4 and resid 344 and name CA)	12.79	0.31	0.31
	assign	(segid 3A4 and resid 19 and name CB)	(segid 3A4 and resid 344 and name CB)	13.08	0.24	0.25
	assign	(segid 3A4 and resid 19 and name CB)	(segid 3A4 and resid 345 and name CA)	11.31	0.61	0.60
	assign	(segid 3A4 and resid 19 and name CB)	(segid 3A4 and resid 345 and name CB)	11.88	0.71	0.71
	assign	(segid 3A4 and resid 19 and name CB)	(segid 3A4 and resid 346 and name CA)	11.38	0.78	0.77
60	assign	(segid 3A4 and resid 19 and name CB)	(segid 3A4 and resid 346 and name CB)	10.64	0.83	0.83
	assign	(segid 3A4 and resid 19 and name CB)	(segid 3A4 and resid 347 and name CA)	13.30	0.81	0.80
	assign	(segid 3A4 and resid 19 and name CB)	(segid 3A4 and resid 347 and name CB)	14.74	0.81	0.81
	assign	(segid 3A4 and resid 19 and name CB)	(segid 3A4 and resid 348 and name CA)	14.04	0.68	0.67
	assign	(segid 3A4 and resid 19 and name CB)	(segid 3A4 and resid 349 and name CA)	10.59	0.68	0.68
65	assign	(segid 3A4 and resid 19 and name CB)	(segid 3A4 and resid 349 and name CB)	9.45	0.65	0.66
	assign	(segid 3A4 and resid 19 and name CB)	(segid 3A4 and resid 34 and name C)	5.56	0.49	0.50
	assign	(segid 3A4 and resid 19 and name CB)	(segid 3A4 and resid 34 and name CA)	5.74	0.44	0.44
	assign	(segid 3A4 and resid 19 and name CB)	(segid 3A4 and resid 34 and name CB)	5.49	0.39	0.39
	assign	(segid 3A4 and resid 19 and name CB)	(segid 3A4 and resid 34 and name N)	5.43	0.43	0.43
70	assign	(segid 3A4 and resid 19 and name CB)	(segid 3A4 and resid 34 and name O)	6.43	0.45	0.45
	assign	(segid 3A4 and resid 19 and name CB)	(segid 3A4 and resid 350 and name CA)	10.47	0.85	0.85
	assign	(segid 3A4 and resid 19 and name CB)	(segid 3A4 and resid 350 and name CB)	10.91	0.91	0.91
	assign	(segid 3A4 and resid 19 and name CB)	(segid 3A4 and resid 351 and name CA)	13.86	0.82	0.83
	assign	(segid 3A4 and resid 19 and name CB)	(segid 3A4 and resid 352 and name CA)	13.11	0.93	0.94
75	assign	(segid 3A4 and resid 19 and name CB)	(segid 3A4 and resid 352 and name CB)	13.29	0.97	0.98
	assign	(segid 3A4 and resid 19 and name CB)	(segid 3A4 and resid 353 and name CA)	10.48	0.97	0.98
	assign	(segid 3A4 and resid 19 and name CB)	(segid 3A4 and resid 353 and name CB)	9.79	0.99	0.99
	assign	(segid 3A4 and resid 19 and name CB)	(segid 3A4 and resid 354 and name CA)	12.46	1.00	1.00
	assign	(segid 3A4 and resid 19 and name CB)	(segid 3A4 and resid 354 and name CB)	12.48	1.03	1.04
80	assign	(segid 3A4 and resid 19 and name CB)	(segid 3A4 and resid 355 and name CA)	11.92	1.22	1.22
	assign	(segid 3A4 and resid 19 and name CB)	(segid 3A4 and resid 355 and name CB)	10.79	1.30	1.30
	assign	(segid 3A4 and resid 19 and name CB)	(segid 3A4 and resid 356 and name CA)	13.66	0.93	0.93
	assign	(segid 3A4 and resid 19 and name CB)	(segid 3A4 and resid 356 and name CB)	13.11	0.87	0.87

	assign (segid 3A4 and resid 19 and name CB) (segid 3A4 and resid 357 and name CA)	16.01	0.94	0.95
	assign (segid 3A4 and resid 19 and name CB) (segid 3A4 and resid 357 and name CB)	16.07	1.00	1.01
	assign (segid 3A4 and resid 19 and name CB) (segid 3A4 and resid 358 and name CA)	17.62	0.85	0.85
	assign (segid 3A4 and resid 19 and name CB) (segid 3A4 and resid 35 and name C)	6.39	0.67	0.66
5	assign (segid 3A4 and resid 19 and name CB) (segid 3A4 and resid 35 and name CA)	5.17	0.64	0.64
	assign (segid 3A4 and resid 19 and name CB) (segid 3A4 and resid 35 and name N)	4.81	0.62	0.63
	assign (segid 3A4 and resid 19 and name CB) (segid 3A4 and resid 35 and name O)	6.67	0.68	0.68
	assign (segid 3A4 and resid 19 and name CB) (segid 3A4 and resid 360 and name CA)	16.90	0.74	0.75
	assign (segid 3A4 and resid 19 and name CB) (segid 3A4 and resid 360 and name CB)	15.39	0.74	0.75
10	assign (segid 3A4 and resid 19 and name CB) (segid 3A4 and resid 36 and name CA)	8.61	0.70	0.70
	assign (segid 3A4 and resid 19 and name CB) (segid 3A4 and resid 37 and name CA)	8.35	0.76	0.77
	assign (segid 3A4 and resid 19 and name CB) (segid 3A4 and resid 37 and name CB)	7.91	0.75	0.75
	assign (segid 3A4 and resid 19 and name CB) (segid 3A4 and resid 381 and name CA)	17.06	0.72	0.71
	assign (segid 3A4 and resid 19 and name CB) (segid 3A4 and resid 382 and name CA)	16.40	0.45	0.46
	assign (segid 3A4 and resid 19 and name CB) (segid 3A4 and resid 383 and name CB)	15.07	0.45	0.46
15	assign (segid 3A4 and resid 19 and name CB) (segid 3A4 and resid 385 and name CA)	18.80	0.41	0.40
	assign (segid 3A4 and resid 19 and name CB) (segid 3A4 and resid 386 and name CA)	18.33	0.49	0.48
	assign (segid 3A4 and resid 19 and name CB) (segid 3A4 and resid 38 and name CA)	18.05	0.50	0.50
	assign (segid 3A4 and resid 19 and name CB) (segid 3A4 and resid 38 and name CB)	6.95	0.92	0.93
20	assign (segid 3A4 and resid 19 and name CB) (segid 3A4 and resid 39 and name CA)	5.68	0.92	0.93
	assign (segid 3A4 and resid 19 and name CB) (segid 3A4 and resid 39 and name CB)	9.42	0.87	0.87
	assign (segid 3A4 and resid 19 and name CB) (segid 3A4 and resid 40 and name CA)	9.62	0.89	0.89
	assign (segid 3A4 and resid 19 and name CB) (segid 3A4 and resid 40 and name CB)	12.13	0.84	0.83
	assign (segid 3A4 and resid 19 and name CB) (segid 3A4 and resid 41 and name CA)	12.38	0.81	0.81
25	assign (segid 3A4 and resid 19 and name CB) (segid 3A4 and resid 41 and name CB)	11.88	0.83	0.84
	assign (segid 3A4 and resid 19 and name CB) (segid 3A4 and resid 42 and name CA)	10.90	0.85	0.84
	assign (segid 3A4 and resid 19 and name CB) (segid 3A4 and resid 42 and name CB)	12.23	0.83	0.84
	assign (segid 3A4 and resid 19 and name CB) (segid 3A4 and resid 19 and name C)	11.37	0.82	0.81
	assign (segid 3A4 and resid 19 and name N) (segid 3A4 and resid 19 and name C)	2.52	0.05	0.05
30	assign (segid 3A4 and resid 19 and name N) (segid 3A4 and resid 19 and name CB)	1.45	0.01	0.02
	assign (segid 3A4 and resid 19 and name N) (segid 3A4 and resid 19 and name O)	2.37	0.04	0.03
	assign (segid 3A4 and resid 19 and name N) (segid 3A4 and resid 20 and name CA)	3.60	0.06	0.05
	assign (segid 3A4 and resid 19 and name N) (segid 3A4 and resid 20 and name CB)	4.72	0.13	0.13
	assign (segid 3A4 and resid 19 and name N) (segid 3A4 and resid 20 and name CA)	4.28	0.10	0.09
35	assign (segid 3A4 and resid 19 and name N) (segid 3A4 and resid 20 and name N)	5.20	0.12	0.12
	assign (segid 3A4 and resid 19 and name N) (segid 3A4 and resid 20 and name O)	2.85	0.09	0.09
	assign (segid 3A4 and resid 19 and name N) (segid 3A4 and resid 21 and name CA)	4.76	0.13	0.13
	assign (segid 3A4 and resid 19 and name N) (segid 3A4 and resid 21 and name CB)	6.34	0.25	0.25
	assign (segid 3A4 and resid 19 and name N) (segid 3A4 and resid 21 and name N)	6.10	0.31	0.30
40	assign (segid 3A4 and resid 19 and name N) (segid 3A4 and resid 21 and name O)	5.49	0.23	0.22
	assign (segid 3A4 and resid 19 and name N) (segid 3A4 and resid 32 and name C)	7.48	0.15	0.14
	assign (segid 3A4 and resid 19 and name N) (segid 3A4 and resid 32 and name O)	6.39	0.12	0.13
	assign (segid 3A4 and resid 19 and name N) (segid 3A4 and resid 34 and name C)	6.56	0.46	0.45
	assign (segid 3A4 and resid 19 and name N) (segid 3A4 and resid 34 and name CA)	6.32	0.42	0.41
45	assign (segid 3A4 and resid 19 and name N) (segid 3A4 and resid 34 and name CB)	5.54	0.43	0.44
	assign (segid 3A4 and resid 19 and name N) (segid 3A4 and resid 34 and name N)	6.07	0.38	0.38
	assign (segid 3A4 and resid 19 and name N) (segid 3A4 and resid 35 and name CA)	6.83	0.60	0.60
	assign (segid 3A4 and resid 19 and name N) (segid 3A4 and resid 35 and name N)	6.20	0.59	0.58
	assign (segid 3A4 and resid 19 and name O) (segid 3A4 and resid 19 and name CB)	3.17	0.11	0.12
50	assign (segid 3A4 and resid 19 and name O) (segid 3A4 and resid 20 and name CA)	4.00	0.09	0.08
	assign (segid 3A4 and resid 19 and name O) (segid 3A4 and resid 20 and name CB)	2.77	0.05	0.04
	assign (segid 3A4 and resid 19 and name O) (segid 3A4 and resid 20 and name N)	3.62	0.18	0.17
	assign (segid 3A4 and resid 19 and name O) (segid 3A4 and resid 20 and name O)	2.23	0.02	0.03
	assign (segid 3A4 and resid 19 and name O) (segid 3A4 and resid 21 and name CA)	4.84	0.03	0.03
55	assign (segid 3A4 and resid 19 and name O) (segid 3A4 and resid 21 and name CB)	6.70	0.24	0.25
	assign (segid 3A4 and resid 19 and name O) (segid 3A4 and resid 21 and name N)	5.82	0.23	0.22
	assign (segid 3A4 and resid 19 and name O) (segid 3A4 and resid 21 and name O)	6.09	0.28	0.28
	assign (segid 3A4 and resid 19 and name O) (segid 3A4 and resid 31 and name C)	4.47	0.22	0.22
60	assign (segid 3A4 and resid 19 and name O) (segid 3A4 and resid 31 and name CA)	6.43	0.27	0.27
	assign (segid 3A4 and resid 19 and name O) (segid 3A4 and resid 32 and name C)	7.37	0.24	0.23
	assign (segid 3A4 and resid 19 and name O) (segid 3A4 and resid 32 and name CA)	4.46	0.19	0.18
	assign (segid 3A4 and resid 19 and name O) (segid 3A4 and resid 32 and name CB)	5.87	0.19	0.19
	assign (segid 3A4 and resid 19 and name O) (segid 3A4 and resid 32 and name N)	6.24	0.23	0.24
65	assign (segid 3A4 and resid 19 and name O) (segid 3A4 and resid 32 and name O)	6.34	0.17	0.18
	assign (segid 3A4 and resid 19 and name O) (segid 3A4 and resid 33 and name CA)	3.61	0.23	0.23
	assign (segid 3A4 and resid 19 and name O) (segid 3A4 and resid 33 and name CB)	3.82	0.32	0.32
	assign (segid 3A4 and resid 19 and name O) (segid 3A4 and resid 33 and name N)	3.69	0.34	0.33
	assign (segid 3A4 and resid 19 and name O) (segid 3A4 and resid 33 and name O)	4.66	0.42	0.43
70	assign (segid 3A4 and resid 19 and name O) (segid 3A4 and resid 33 and name CA)	4.54	0.23	0.24
	assign (segid 3A4 and resid 19 and name O) (segid 3A4 and resid 34 and name C)	5.01	0.32	0.31
	assign (segid 3A4 and resid 19 and name O) (segid 3A4 and resid 34 and name CA)	4.51	0.19	0.19
	assign (segid 3A4 and resid 19 and name O) (segid 3A4 and resid 34 and name CB)	3.92	0.18	0.17
	assign (segid 3A4 and resid 19 and name O) (segid 3A4 and resid 34 and name N)	3.88	0.16	0.16
	assign (segid 3A4 and resid 19 and name O) (segid 3A4 and resid 34 and name O)	3.03	0.26	0.26
75	assign (segid 3A4 and resid 19 and name O) (segid 3A4 and resid 35 and name C)	5.64	0.16	0.17
	assign (segid 3A4 and resid 19 and name O) (segid 3A4 and resid 35 and name CA)	6.30	0.35	0.34
	assign (segid 3A4 and resid 19 and name O) (segid 3A4 and resid 35 and name N)	5.29	0.30	0.31
	assign (segid 3A4 and resid 19 and name O) (segid 3A4 and resid 35 and name O)	4.18	0.28	0.29
80	assign (segid 3A4 and resid 19 and name O) (segid 3A4 and resid 38 and name CA)	6.15	0.42	0.41
	assign (segid 3A4 and resid 19 and name O) (segid 3A4 and resid 38 and name CB)	6.62	0.59	0.60
	assign (segid 3A4 and resid 19 and name O) (segid 3A4 and resid 38 and name N)	5.19	0.60	0.61
	assign (segid 3A4 and resid 19 and name O) (segid 3A4 and resid 200 and name O)	7.08	0.49	0.49
	assign (segid 3A4 and resid 200 and name C) (segid 3A4 and resid 200 and name O)	1.23	0.00	0.00

	assign	(segid 3A4 and resid 200 and name C)	(segid 3A4 and resid 201 and name C)	3.04	0.07	0.07
	assign	(segid 3A4 and resid 200 and name C)	(segid 3A4 and resid 201 and name CA)	2.44	0.01	0.01
	assign	(segid 3A4 and resid 200 and name C)	(segid 3A4 and resid 201 and name CB)	3.73	0.04	0.03
	assign	(segid 3A4 and resid 200 and name C)	(segid 3A4 and resid 201 and name N)	1.33	0.00	0.01
5	assign	(segid 3A4 and resid 200 and name C)	(segid 3A4 and resid 201 and name O)	3.87	0.10	0.10
	assign	(segid 3A4 and resid 200 and name C)	(segid 3A4 and resid 202 and name C)	4.63	0.12	0.13
	assign	(segid 3A4 and resid 200 and name C)	(segid 3A4 and resid 202 and name CA)	4.54	0.11	0.11
	assign	(segid 3A4 and resid 200 and name C)	(segid 3A4 and resid 202 and name CB)	5.28	0.08	0.09
	assign	(segid 3A4 and resid 200 and name C)	(segid 3A4 and resid 202 and name CG1)	6.55	0.09	0.09
10	assign	(segid 3A4 and resid 200 and name C)	(segid 3A4 and resid 202 and name N)	3.35	0.10	0.10
	assign	(segid 3A4 and resid 200 and name C)	(segid 3A4 and resid 202 and name O)	5.70	0.12	0.12
	assign	(segid 3A4 and resid 200 and name C)	(segid 3A4 and resid 203 and name C)	4.97	0.09	0.09
	assign	(segid 3A4 and resid 200 and name C)	(segid 3A4 and resid 203 and name CA)	4.62	0.13	0.12
	assign	(segid 3A4 and resid 200 and name C)	(segid 3A4 and resid 203 and name CB)	4.36	0.13	0.13
15	assign	(segid 3A4 and resid 200 and name C)	(segid 3A4 and resid 203 and name N)	3.91	0.13	0.13
	assign	(segid 3A4 and resid 200 and name C)	(segid 3A4 and resid 203 and name O)	6.18	0.08	0.09
	assign	(segid 3A4 and resid 200 and name C)	(segid 3A4 and resid 204 and name C)	6.12	0.11	0.10
	assign	(segid 3A4 and resid 200 and name C)	(segid 3A4 and resid 204 and name CA)	5.10	0.12	0.11
	assign	(segid 3A4 and resid 200 and name C)	(segid 3A4 and resid 204 and name CB)	4.67	0.20	0.21
20	assign	(segid 3A4 and resid 200 and name C)	(segid 3A4 and resid 204 and name N)	4.22	0.08	0.08
	assign	(segid 3A4 and resid 200 and name C)	(segid 3A4 and resid 204 and name O)	7.27	0.10	0.10
	assign	(segid 3A4 and resid 200 and name C)	(segid 3A4 and resid 205 and name C)	7.19	0.14	0.14
	assign	(segid 3A4 and resid 200 and name C)	(segid 3A4 and resid 205 and name CB)	7.14	0.19	0.19
	assign	(segid 3A4 and resid 200 and name C)	(segid 3A4 and resid 205 and name N)	5.96	0.13	0.12
25	assign	(segid 3A4 and resid 200 and name C)	(segid 3A4 and resid 206 and name N)	7.89	0.09	0.08
	assign	(segid 3A4 and resid 200 and name C)	(segid 3A4 and resid 200 and name C)	1.52	0.01	0.01
	assign	(segid 3A4 and resid 200 and name CA)	(segid 3A4 and resid 200 and name O)	2.38	0.02	0.02
	assign	(segid 3A4 and resid 200 and name CA)	(segid 3A4 and resid 201 and name C)	4.40	0.03	0.04
	assign	(segid 3A4 and resid 200 and name CA)	(segid 3A4 and resid 201 and name CA)	3.81	0.03	0.02
30	assign	(segid 3A4 and resid 200 and name CA)	(segid 3A4 and resid 201 and name CB)	4.87	0.06	0.06
	assign	(segid 3A4 and resid 200 and name CA)	(segid 3A4 and resid 201 and name N)	2.44	0.04	0.03
	assign	(segid 3A4 and resid 200 and name CA)	(segid 3A4 and resid 201 and name O)	5.31	0.08	0.09
	assign	(segid 3A4 and resid 200 and name CA)	(segid 3A4 and resid 202 and name C)	5.57	0.09	0.08
	assign	(segid 3A4 and resid 200 and name CA)	(segid 3A4 and resid 202 and name CA)	5.50	0.06	0.05
35	assign	(segid 3A4 and resid 200 and name CA)	(segid 3A4 and resid 202 and name CB)	5.90	0.06	0.06
	assign	(segid 3A4 and resid 200 and name CA)	(segid 3A4 and resid 202 and name CG1)	7.12	0.04	0.03
	assign	(segid 3A4 and resid 200 and name CA)	(segid 3A4 and resid 202 and name N)	4.41	0.06	0.05
	assign	(segid 3A4 and resid 200 and name CA)	(segid 3A4 and resid 202 and name O)	6.69	0.09	0.09
	assign	(segid 3A4 and resid 200 and name CA)	(segid 3A4 and resid 203 and name C)	5.82	0.13	0.12
40	assign	(segid 3A4 and resid 200 and name CA)	(segid 3A4 and resid 203 and name CA)	5.21	0.12	0.12
	assign	(segid 3A4 and resid 200 and name CA)	(segid 3A4 and resid 203 and name CB)	4.55	0.14	0.15
	assign	(segid 3A4 and resid 200 and name CA)	(segid 3A4 and resid 203 and name N)	4.64	0.10	0.10
	assign	(segid 3A4 and resid 200 and name CA)	(segid 3A4 and resid 203 and name O)	7.01	0.12	0.13
	assign	(segid 3A4 and resid 200 and name CA)	(segid 3A4 and resid 204 and name C)	7.39	0.15	0.14
45	assign	(segid 3A4 and resid 200 and name CA)	(segid 3A4 and resid 204 and name CA)	6.24	0.17	0.17
	assign	(segid 3A4 and resid 200 and name CA)	(segid 3A4 and resid 204 and name CB)	5.90	0.21	0.21
	assign	(segid 3A4 and resid 200 and name CA)	(segid 3A4 and resid 204 and name N)	5.25	0.13	0.14
	assign	(segid 3A4 and resid 200 and name CA)	(segid 3A4 and resid 205 and name C)	8.56	0.15	0.15
	assign	(segid 3A4 and resid 200 and name CA)	(segid 3A4 and resid 205 and name CA)	8.54	0.20	0.19
	assign	(segid 3A4 and resid 200 and name CA)	(segid 3A4 and resid 205 and name CB)	7.30	0.15	0.14
50	assign	(segid 3A4 and resid 200 and name CA)	(segid 3A4 and resid 206 and name C)	10.06	0.07	0.07
	assign	(segid 3A4 and resid 200 and name CA)	(segid 3A4 and resid 206 and name CB)	9.67	0.10	0.10
	assign	(segid 3A4 and resid 200 and name CA)	(segid 3A4 and resid 207 and name CA)	11.07	0.31	0.32
	assign	(segid 3A4 and resid 200 and name CA)	(segid 3A4 and resid 207 and name CB)	10.44	0.44	0.43
	assign	(segid 3A4 and resid 200 and name CA)	(segid 3A4 and resid 207 and name N)	15.42	0.34	0.35
55	assign	(segid 3A4 and resid 200 and name CA)	(segid 3A4 and resid 219 and name CA)	14.27	0.28	0.27
	assign	(segid 3A4 and resid 200 and name CA)	(segid 3A4 and resid 219 and name CB)	15.10	0.52	0.51
	assign	(segid 3A4 and resid 200 and name CA)	(segid 3A4 and resid 220 and name CA)	15.32	0.61	0.62
	assign	(segid 3A4 and resid 200 and name CA)	(segid 3A4 and resid 220 and name CB)	11.63	0.56	0.56
	assign	(segid 3A4 and resid 200 and name CA)	(segid 3A4 and resid 221 and name CA)	10.35	0.51	0.51
60	assign	(segid 3A4 and resid 200 and name CA)	(segid 3A4 and resid 221 and name CB)	12.96	0.77	0.77
	assign	(segid 3A4 and resid 200 and name CA)	(segid 3A4 and resid 222 and name CA)	13.63	0.76	0.77
	assign	(segid 3A4 and resid 200 and name CA)	(segid 3A4 and resid 222 and name CB)	16.09	0.73	0.74
	assign	(segid 3A4 and resid 200 and name CA)	(segid 3A4 and resid 223 and name CA)	17.01	0.69	0.70
	assign	(segid 3A4 and resid 200 and name CA)	(segid 3A4 and resid 223 and name CB)	14.73	0.71	0.72
65	assign	(segid 3A4 and resid 200 and name CA)	(segid 3A4 and resid 224 and name CA)	14.00	0.59	0.59
	assign	(segid 3A4 and resid 200 and name CA)	(segid 3A4 and resid 224 and name CB)	12.78	1.12	1.12
	assign	(segid 3A4 and resid 200 and name CA)	(segid 3A4 and resid 225 and name CA)	11.73	1.17	1.17
	assign	(segid 3A4 and resid 200 and name CA)	(segid 3A4 and resid 225 and name CB)	16.02	1.31	1.31
	assign	(segid 3A4 and resid 200 and name CA)	(segid 3A4 and resid 226 and name CA)	14.76	0.59	0.59
70	assign	(segid 3A4 and resid 200 and name CA)	(segid 3A4 and resid 240 and name CA)	15.47	0.65	0.66
	assign	(segid 3A4 and resid 200 and name CA)	(segid 3A4 and resid 240 and name CB)	11.12	0.65	0.64
	assign	(segid 3A4 and resid 200 and name CA)	(segid 3A4 and resid 241 and name CA)	10.47	0.78	0.78
	assign	(segid 3A4 and resid 200 and name CA)	(segid 3A4 and resid 241 and name CB)	12.26	0.81	0.82
	assign	(segid 3A4 and resid 200 and name CA)	(segid 3A4 and resid 242 and name CA)	13.33	0.91	0.92
75	assign	(segid 3A4 and resid 200 and name CA)	(segid 3A4 and resid 242 and name CB)	14.42	0.50	0.51
	assign	(segid 3A4 and resid 200 and name CA)	(segid 3A4 and resid 243 and name CA)	15.57	0.50	0.49
	assign	(segid 3A4 and resid 200 and name CA)	(segid 3A4 and resid 243 and name CB)	12.05	0.33	0.33
	assign	(segid 3A4 and resid 200 and name CA)	(segid 3A4 and resid 244 and name CA)	11.28	0.40	0.40
	assign	(segid 3A4 and resid 200 and name CA)	(segid 3A4 and resid 244 and name CB)	10.01	0.36	0.35
80	assign	(segid 3A4 and resid 200 and name CA)	(segid 3A4 and resid 245 and name CA)	9.45	0.42	0.43
	assign	(segid 3A4 and resid 200 and name CA)	(segid 3A4 and resid 245 and name CB)	13.46	0.48	0.48
	assign	(segid 3A4 and resid 200 and name CA)	(segid 3A4 and resid 246 and name CA)	14.54	0.48	0.49
	assign	(segid 3A4 and resid 200 and name CA)	(segid 3A4 and resid 246 and name CB)			

	assign (segid 3A4 and resid 200 and name CA)	(segid 3A4 and resid 247 and name CA)	14.73	0.21	0.20
	assign (segid 3A4 and resid 200 and name CA)	(segid 3A4 and resid 247 and name CB)	14.97	0.17	0.18
	assign (segid 3A4 and resid 200 and name CA)	(segid 3A4 and resid 248 and name CA)	12.23	0.33	0.33
	assign (segid 3A4 and resid 200 and name CA)	(segid 3A4 and resid 248 and name CB)	10.79	0.30	0.30
5	assign (segid 3A4 and resid 200 and name CA)	(segid 3A4 and resid 249 and name CA)	13.04	0.76	0.77
	assign (segid 3A4 and resid 200 and name CA)	(segid 3A4 and resid 250 and name CA)	16.60	0.66	0.66
	assign (segid 3A4 and resid 200 and name CA)	(segid 3A4 and resid 250 and name CB)	17.29	0.52	0.52
	assign (segid 3A4 and resid 200 and name CA)	(segid 3A4 and resid 251 and name CA)	16.78	0.57	0.57
	assign (segid 3A4 and resid 200 and name CA)	(segid 3A4 and resid 251 and name CB)	16.16	0.46	0.45
10	assign (segid 3A4 and resid 200 and name CA)	(segid 3A4 and resid 252 and name CA)	15.62	0.89	0.89
	assign (segid 3A4 and resid 200 and name CA)	(segid 3A4 and resid 252 and name CB)	14.30	0.94	0.94
	assign (segid 3A4 and resid 200 and name CA)	(segid 3A4 and resid 253 and name CA)	17.98	0.96	0.97
	assign (segid 3A4 and resid 200 and name N)	(segid 3A4 and resid 200 and name C)	2.44	0.02	0.02
	assign (segid 3A4 and resid 200 and name N)	(segid 3A4 and resid 200 and name CA)	1.45	0.00	0.01
15	assign (segid 3A4 and resid 200 and name N)	(segid 3A4 and resid 200 and name O)	3.49	0.04	0.03
	assign (segid 3A4 and resid 200 and name N)	(segid 3A4 and resid 201 and name C)	4.66	0.06	0.06
	assign (segid 3A4 and resid 200 and name N)	(segid 3A4 and resid 201 and name CA)	4.17	0.08	0.08
	assign (segid 3A4 and resid 200 and name N)	(segid 3A4 and resid 201 and name CB)	4.92	0.11	0.10
	assign (segid 3A4 and resid 200 and name N)	(segid 3A4 and resid 201 and name N)	2.77	0.08	0.09
20	assign (segid 3A4 and resid 200 and name N)	(segid 3A4 and resid 201 and name O)	5.75	0.07	0.06
	assign (segid 3A4 and resid 200 and name N)	(segid 3A4 and resid 202 and name C)	5.68	0.06	0.06
	assign (segid 3A4 and resid 200 and name N)	(segid 3A4 and resid 202 and name CA)	5.33	0.07	0.07
	assign (segid 3A4 and resid 200 and name N)	(segid 3A4 and resid 202 and name CB)	5.38	0.09	0.10
	assign (segid 3A4 and resid 200 and name N)	(segid 3A4 and resid 202 and name CG1)	6.64	0.05	0.05
25	assign (segid 3A4 and resid 200 and name N)	(segid 3A4 and resid 202 and name N)	4.30	0.08	0.08
	assign (segid 3A4 and resid 200 and name N)	(segid 3A4 and resid 202 and name O)	6.89	0.06	0.06
	assign (segid 3A4 and resid 200 and name N)	(segid 3A4 and resid 203 and name C)	6.56	0.08	0.08
	assign (segid 3A4 and resid 200 and name N)	(segid 3A4 and resid 203 and name CA)	5.69	0.09	0.09
	assign (segid 3A4 and resid 200 and name N)	(segid 3A4 and resid 203 and name CB)	5.14	0.13	0.13
30	assign (segid 3A4 and resid 200 and name N)	(segid 3A4 and resid 203 and name N)	4.89	0.07	0.08
	assign (segid 3A4 and resid 200 and name N)	(segid 3A4 and resid 203 and name O)	7.76	0.07	0.08
	assign (segid 3A4 and resid 200 and name N)	(segid 3A4 and resid 204 and name CA)	7.28	0.13	0.12
	assign (segid 3A4 and resid 200 and name N)	(segid 3A4 and resid 204 and name CB)	7.04	0.20	0.20
	assign (segid 3A4 and resid 200 and name N)	(segid 3A4 and resid 204 and name N)	6.16	0.09	0.10
35	assign (segid 3A4 and resid 200 and name O)	(segid 3A4 and resid 201 and name C)	3.03	0.16	0.15
	assign (segid 3A4 and resid 200 and name O)	(segid 3A4 and resid 201 and name CA)	2.78	0.01	0.01
	assign (segid 3A4 and resid 200 and name O)	(segid 3A4 and resid 201 and name CB)	4.26	0.03	0.04
	assign (segid 3A4 and resid 200 and name O)	(segid 3A4 and resid 201 and name N)	2.25	0.01	0.01
	assign (segid 3A4 and resid 200 and name O)	(segid 3A4 and resid 201 and name O)	3.49	0.17	0.18
40	assign (segid 3A4 and resid 200 and name O)	(segid 3A4 and resid 202 and name C)	4.25	0.26	0.27
	assign (segid 3A4 and resid 200 and name O)	(segid 3A4 and resid 202 and name CA)	4.52	0.25	0.25
	assign (segid 3A4 and resid 200 and name O)	(segid 3A4 and resid 202 and name CB)	5.48	0.21	0.22
	assign (segid 3A4 and resid 200 and name O)	(segid 3A4 and resid 202 and name CG1)	6.59	0.25	0.24
	assign (segid 3A4 and resid 200 and name O)	(segid 3A4 and resid 202 and name N)	3.54	0.22	0.22
45	assign (segid 3A4 and resid 200 and name O)	(segid 3A4 and resid 202 and name O)	5.16	0.27	0.27
	assign (segid 3A4 and resid 200 and name O)	(segid 3A4 and resid 203 and name C)	3.98	0.18	0.18
	assign (segid 3A4 and resid 200 and name O)	(segid 3A4 and resid 203 and name CA)	3.89	0.23	0.22
	assign (segid 3A4 and resid 200 and name O)	(segid 3A4 and resid 203 and name CB)	3.70	0.20	0.19
	assign (segid 3A4 and resid 200 and name O)	(segid 3A4 and resid 203 and name N)	3.45	0.24	0.25
50	assign (segid 3A4 and resid 200 and name O)	(segid 3A4 and resid 203 and name O)	5.16	0.17	0.16
	assign (segid 3A4 and resid 200 and name O)	(segid 3A4 and resid 204 and name C)	5.07	0.15	0.15
	assign (segid 3A4 and resid 200 and name O)	(segid 3A4 and resid 204 and name CA)	3.95	0.13	0.13
	assign (segid 3A4 and resid 200 and name O)	(segid 3A4 and resid 204 and name CB)	3.61	0.20	0.20
	assign (segid 3A4 and resid 200 and name O)	(segid 3A4 and resid 204 and name N)	3.12	0.15	0.15
55	assign (segid 3A4 and resid 200 and name O)	(segid 3A4 and resid 204 and name O)	6.20	0.14	0.13
	assign (segid 3A4 and resid 200 and name O)	(segid 3A4 and resid 205 and name C)	7.35	0.20	0.20
	assign (segid 3A4 and resid 200 and name O)	(segid 3A4 and resid 205 and name CA)	6.39	0.22	0.23
	assign (segid 3A4 and resid 200 and name O)	(segid 3A4 and resid 205 and name CB)	6.56	0.27	0.28
	assign (segid 3A4 and resid 200 and name O)	(segid 3A4 and resid 205 and name N)	5.07	0.21	0.21
60	assign (segid 3A4 and resid 200 and name O)	(segid 3A4 and resid 206 and name N)	7.03	0.17	0.18
	assign (segid 3A4 and resid 201 and name C)	(segid 3A4 and resid 201 and name CB)	2.51	0.04	0.03
	assign (segid 3A4 and resid 201 and name C)	(segid 3A4 and resid 201 and name O)	1.23	0.00	0.01
	assign (segid 3A4 and resid 201 and name C)	(segid 3A4 and resid 202 and name C)	3.02	0.05	0.05
	assign (segid 3A4 and resid 201 and name C)	(segid 3A4 and resid 202 and name CA)	2.45	0.02	0.03
65	assign (segid 3A4 and resid 201 and name C)	(segid 3A4 and resid 202 and name CB)	3.74	0.01	0.01
	assign (segid 3A4 and resid 201 and name C)	(segid 3A4 and resid 202 and name CG1)	4.97	0.03	0.02
	assign (segid 3A4 and resid 201 and name C)	(segid 3A4 and resid 202 and name N)	1.33	0.01	0.01
	assign (segid 3A4 and resid 201 and name C)	(segid 3A4 and resid 202 and name O)	3.86	0.05	0.04
	assign (segid 3A4 and resid 201 and name C)	(segid 3A4 and resid 203 and name C)	4.56	0.07	0.06
70	assign (segid 3A4 and resid 201 and name C)	(segid 3A4 and resid 203 and name CA)	4.46	0.07	0.06
	assign (segid 3A4 and resid 201 and name C)	(segid 3A4 and resid 203 and name CB)	5.17	0.06	0.07
	assign (segid 3A4 and resid 201 and name C)	(segid 3A4 and resid 203 and name N)	3.28	0.08	0.08
	assign (segid 3A4 and resid 201 and name C)	(segid 3A4 and resid 203 and name O)	5.60	0.08	0.07
	assign (segid 3A4 and resid 201 and name C)	(segid 3A4 and resid 204 and name C)	4.83	0.08	0.07
75	assign (segid 3A4 and resid 201 and name C)	(segid 3A4 and resid 204 and name CA)	4.57	0.11	0.11
	assign (segid 3A4 and resid 201 and name C)	(segid 3A4 and resid 204 and name CB)	4.38	0.23	0.24
	assign (segid 3A4 and resid 201 and name C)	(segid 3A4 and resid 204 and name N)	3.86	0.08	0.09
	assign (segid 3A4 and resid 201 and name C)	(segid 3A4 and resid 204 and name O)	6.01	0.08	0.08
	assign (segid 3A4 and resid 201 and name C)	(segid 3A4 and resid 205 and name C)	6.00	0.08	0.09
80	assign (segid 3A4 and resid 201 and name C)	(segid 3A4 and resid 205 and name CA)	4.90	0.11	0.12
	assign (segid 3A4 and resid 201 and name C)	(segid 3A4 and resid 205 and name CB)	4.43	0.17	0.17
	assign (segid 3A4 and resid 201 and name C)	(segid 3A4 and resid 205 and name N)	4.08	0.08	0.07
	assign (segid 3A4 and resid 201 and name C)	(segid 3A4 and resid 205 and name O)	7.09	0.11	0.11

	assign (segid 3A4 and resid 201 and name C)	(segid 3A4 and resid 206 and name CA)	7.28	0.09	0.10
	assign (segid 3A4 and resid 201 and name C)	(segid 3A4 and resid 206 and name CB)	7.37	0.14	0.14
	assign (segid 3A4 and resid 201 and name C)	(segid 3A4 and resid 206 and name N)	5.98	0.07	0.08
	assign (segid 3A4 and resid 201 and name C)	(segid 3A4 and resid 221 and name CB)	6.27	0.47	0.47
5	assign (segid 3A4 and resid 201 and name CA)	(segid 3A4 and resid 201 and name C)	1.52	0.01	0.01
	assign (segid 3A4 and resid 201 and name CA)	(segid 3A4 and resid 201 and name CB)	1.55	0.03	0.02
	assign (segid 3A4 and resid 201 and name CA)	(segid 3A4 and resid 201 and name O)	2.39	0.02	0.01
	assign (segid 3A4 and resid 201 and name CA)	(segid 3A4 and resid 202 and name C)	4.42	0.05	0.06
	assign (segid 3A4 and resid 201 and name CA)	(segid 3A4 and resid 202 and name CA)	3.83	0.03	0.03
10	assign (segid 3A4 and resid 201 and name CA)	(segid 3A4 and resid 202 and name CB)	4.89	0.02	0.01
	assign (segid 3A4 and resid 201 and name CA)	(segid 3A4 and resid 202 and name CG1)	6.25	0.02	0.03
	assign (segid 3A4 and resid 201 and name CA)	(segid 3A4 and resid 202 and name N)	2.44	0.02	0.03
	assign (segid 3A4 and resid 201 and name CA)	(segid 3A4 and resid 202 and name O)	5.32	0.05	0.05
	assign (segid 3A4 and resid 201 and name CA)	(segid 3A4 and resid 203 and name C)	5.53	0.09	0.08
15	assign (segid 3A4 and resid 201 and name CA)	(segid 3A4 and resid 203 and name CA)	5.46	0.08	0.08
	assign (segid 3A4 and resid 201 and name CA)	(segid 3A4 and resid 203 and name CB)	5.84	0.09	0.10
	assign (segid 3A4 and resid 201 and name CA)	(segid 3A4 and resid 203 and name N)	4.40	0.09	0.09
	assign (segid 3A4 and resid 201 and name CA)	(segid 3A4 and resid 203 and name O)	6.63	0.09	0.09
20	assign (segid 3A4 and resid 201 and name CA)	(segid 3A4 and resid 204 and name C)	5.66	0.12	0.12
	assign (segid 3A4 and resid 201 and name CA)	(segid 3A4 and resid 204 and name CA)	5.16	0.14	0.14
	assign (segid 3A4 and resid 201 and name CA)	(segid 3A4 and resid 204 and name CB)	4.55	0.24	0.25
	assign (segid 3A4 and resid 201 and name CA)	(segid 3A4 and resid 204 and name N)	4.62	0.10	0.10
	assign (segid 3A4 and resid 201 and name CA)	(segid 3A4 and resid 204 and name O)	6.80	0.13	0.13
25	assign (segid 3A4 and resid 201 and name CA)	(segid 3A4 and resid 205 and name C)	7.28	0.10	0.10
	assign (segid 3A4 and resid 201 and name CA)	(segid 3A4 and resid 205 and name CA)	6.05	0.13	0.13
	assign (segid 3A4 and resid 201 and name CA)	(segid 3A4 and resid 205 and name CB)	5.63	0.15	0.15
	assign (segid 3A4 and resid 201 and name CA)	(segid 3A4 and resid 205 and name N)	5.14	0.11	0.10
	assign (segid 3A4 and resid 201 and name CA)	(segid 3A4 and resid 206 and name CA)	8.66	0.11	0.12
	assign (segid 3A4 and resid 201 and name CA)	(segid 3A4 and resid 206 and name CB)	8.77	0.16	0.15
30	assign (segid 3A4 and resid 201 and name CA)	(segid 3A4 and resid 206 and name N)	7.33	0.10	0.10
	assign (segid 3A4 and resid 201 and name CA)	(segid 3A4 and resid 207 and name CA)	10.12	0.06	0.06
	assign (segid 3A4 and resid 201 and name CA)	(segid 3A4 and resid 207 and name CB)	9.86	0.16	0.15
	assign (segid 3A4 and resid 201 and name CA)	(segid 3A4 and resid 219 and name CA)	11.70	0.36	0.37
35	assign (segid 3A4 and resid 201 and name CA)	(segid 3A4 and resid 219 and name CB)	10.51	0.28	0.28
	assign (segid 3A4 and resid 201 and name CA)	(segid 3A4 and resid 220 and name CA)	11.66	0.51	0.52
	assign (segid 3A4 and resid 201 and name CA)	(segid 3A4 and resid 220 and name CB)	11.98	0.54	0.54
	assign (segid 3A4 and resid 201 and name CA)	(segid 3A4 and resid 221 and name CA)	8.38	0.62	0.62
	assign (segid 3A4 and resid 201 and name CA)	(segid 3A4 and resid 221 and name CB)	6.99	0.56	0.55
40	assign (segid 3A4 and resid 201 and name CA)	(segid 3A4 and resid 222 and name CA)	9.75	0.84	0.83
	assign (segid 3A4 and resid 201 and name CA)	(segid 3A4 and resid 222 and name CB)	10.30	0.81	0.82
	assign (segid 3A4 and resid 201 and name CA)	(segid 3A4 and resid 223 and name CA)	13.02	0.80	0.80
	assign (segid 3A4 and resid 201 and name CA)	(segid 3A4 and resid 223 and name CB)	13.83	0.76	0.76
	assign (segid 3A4 and resid 201 and name CA)	(segid 3A4 and resid 224 and name CA)	12.20	0.76	0.76
45	assign (segid 3A4 and resid 201 and name CA)	(segid 3A4 and resid 224 and name CB)	11.52	0.59	0.59
	assign (segid 3A4 and resid 201 and name CA)	(segid 3A4 and resid 225 and name CA)	10.67	1.14	1.14
	assign (segid 3A4 and resid 201 and name CA)	(segid 3A4 and resid 225 and name CB)	9.52	1.21	1.21
	assign (segid 3A4 and resid 201 and name CA)	(segid 3A4 and resid 226 and name CA)	13.82	1.29	1.29
	assign (segid 3A4 and resid 201 and name CA)	(segid 3A4 and resid 240 and name CA)	14.67	0.45	0.46
50	assign (segid 3A4 and resid 201 and name CA)	(segid 3A4 and resid 240 and name CB)	15.65	0.49	0.48
	assign (segid 3A4 and resid 201 and name CA)	(segid 3A4 and resid 241 and name CA)	11.33	0.58	0.59
	assign (segid 3A4 and resid 201 and name CA)	(segid 3A4 and resid 241 and name CB)	11.10	0.72	0.72
	assign (segid 3A4 and resid 201 and name CA)	(segid 3A4 and resid 242 and name CA)	12.81	0.68	0.68
	assign (segid 3A4 and resid 201 and name CA)	(segid 3A4 and resid 242 and name CB)	14.13	0.72	0.73
55	assign (segid 3A4 and resid 201 and name CA)	(segid 3A4 and resid 243 and name CA)	14.03	0.43	0.44
	assign (segid 3A4 and resid 201 and name CA)	(segid 3A4 and resid 243 and name CB)	15.05	0.42	0.42
	assign (segid 3A4 and resid 201 and name CA)	(segid 3A4 and resid 244 and name CA)	10.94	0.37	0.36
	assign (segid 3A4 and resid 201 and name CA)	(segid 3A4 and resid 244 and name CB)	10.13	0.42	0.41
	assign (segid 3A4 and resid 201 and name CA)	(segid 3A4 and resid 245 and name CA)	9.51	0.43	0.42
60	assign (segid 3A4 and resid 201 and name CA)	(segid 3A4 and resid 245 and name CB)	9.54	0.44	0.45
	assign (segid 3A4 and resid 201 and name CA)	(segid 3A4 and resid 246 and name CA)	12.94	0.55	0.55
	assign (segid 3A4 and resid 201 and name CA)	(segid 3A4 and resid 246 and name CB)	14.21	0.52	0.51
	assign (segid 3A4 and resid 201 and name CA)	(segid 3A4 and resid 247 and name CA)	13.22	0.37	0.37
	assign (segid 3A4 and resid 201 and name CA)	(segid 3A4 and resid 247 and name CB)	13.29	0.33	0.32
65	assign (segid 3A4 and resid 201 and name CA)	(segid 3A4 and resid 248 and name CA)	10.30	0.51	0.52
	assign (segid 3A4 and resid 201 and name CA)	(segid 3A4 and resid 248 and name CB)	8.85	0.47	0.47
	assign (segid 3A4 and resid 201 and name CA)	(segid 3A4 and resid 249 and name CA)	11.91	0.93	0.92
	assign (segid 3A4 and resid 201 and name CA)	(segid 3A4 and resid 250 and name CA)	15.17	0.81	0.80
	assign (segid 3A4 and resid 201 and name CA)	(segid 3A4 and resid 250 and name CB)	15.87	0.66	0.66
70	assign (segid 3A4 and resid 201 and name CA)	(segid 3A4 and resid 251 and name CA)	14.56	0.73	0.73
	assign (segid 3A4 and resid 201 and name CA)	(segid 3A4 and resid 251 and name CB)	13.72	0.60	0.61
	assign (segid 3A4 and resid 201 and name CA)	(segid 3A4 and resid 252 and name CA)	13.60	1.08	1.07
	assign (segid 3A4 and resid 201 and name CA)	(segid 3A4 and resid 252 and name CB)	12.46	1.14	1.14
	assign (segid 3A4 and resid 201 and name CA)	(segid 3A4 and resid 253 and name CA)	16.53	1.12	1.12
	assign (segid 3A4 and resid 201 and name CA)	(segid 3A4 and resid 254 and name CA)	18.93	0.95	0.96
75	assign (segid 3A4 and resid 201 and name CB)	(segid 3A4 and resid 202 and name C)	5.43	0.04	0.03
	assign (segid 3A4 and resid 201 and name CB)	(segid 3A4 and resid 202 and name CA)	4.47	0.06	0.07
	assign (segid 3A4 and resid 201 and name CB)	(segid 3A4 and resid 202 and name CB)	5.34	0.11	0.10
	assign (segid 3A4 and resid 201 and name CB)	(segid 3A4 and resid 202 and name CG1)	6.76	0.11	0.11
80	assign (segid 3A4 and resid 201 and name CB)	(segid 3A4 and resid 202 and name N)	3.14	0.06	0.06
	assign (segid 3A4 and resid 201 and name CB)	(segid 3A4 and resid 202 and name O)	6.28	0.07	0.07
	assign (segid 3A4 and resid 201 and name CB)	(segid 3A4 and resid 203 and name C)	6.93	0.08	0.09
	assign (segid 3A4 and resid 201 and name CB)	(segid 3A4 and resid 203 and name CA)	6.82	0.05	0.05
	assign (segid 3A4 and resid 201 and name CB)	(segid 3A4 and resid 203 and name CB)	7.28	0.05	0.05

	assign (segid 3A4 and resid 201 and name CB)	(segid 3A4 and resid 203 and name N)	5.63	0.05	0.05
	assign (segid 3A4 and resid 201 and name CB)	(segid 3A4 and resid 204 and name C)	6.81	0.17	0.17
	assign (segid 3A4 and resid 201 and name CB)	(segid 3A4 and resid 204 and name CA)	6.51	0.17	0.17
	assign (segid 3A4 and resid 201 and name CB)	(segid 3A4 and resid 204 and name CB)	5.82	0.27	0.28
	assign (segid 3A4 and resid 201 and name CB)	(segid 3A4 and resid 204 and name N)	6.06	0.12	0.11
5	assign (segid 3A4 and resid 201 and name CB)	(segid 3A4 and resid 205 and name CA)	6.80	0.17	0.17
	assign (segid 3A4 and resid 201 and name CB)	(segid 3A4 and resid 205 and name CB)	6.09	0.17	0.18
	assign (segid 3A4 and resid 201 and name CB)	(segid 3A4 and resid 205 and name N)	6.14	0.15	0.15
	assign (segid 3A4 and resid 201 and name CB)	(segid 3A4 and resid 206 and name CA)	9.64	0.11	0.11
	assign (segid 3A4 and resid 201 and name CB)	(segid 3A4 and resid 206 and name CB)	9.82	0.12	0.12
10	assign (segid 3A4 and resid 201 and name CB)	(segid 3A4 and resid 207 and name CA)	11.33	0.04	0.03
	assign (segid 3A4 and resid 201 and name CB)	(segid 3A4 and resid 207 and name CB)	11.16	0.10	0.11
	assign (segid 3A4 and resid 201 and name CB)	(segid 3A4 and resid 219 and name CA)	10.95	0.39	0.39
	assign (segid 3A4 and resid 201 and name CB)	(segid 3A4 and resid 219 and name CB)	9.72	0.30	0.31
	assign (segid 3A4 and resid 201 and name CB)	(segid 3A4 and resid 220 and name CA)	10.79	0.54	0.54
15	assign (segid 3A4 and resid 201 and name CB)	(segid 3A4 and resid 220 and name CB)	10.96	0.55	0.56
	assign (segid 3A4 and resid 201 and name CB)	(segid 3A4 and resid 221 and name CA)	7.72	0.67	0.68
	assign (segid 3A4 and resid 201 and name CB)	(segid 3A4 and resid 221 and name CB)	6.28	0.63	0.62
	assign (segid 3A4 and resid 201 and name CB)	(segid 3A4 and resid 222 and name CA)	9.58	0.80	0.81
	assign (segid 3A4 and resid 201 and name CB)	(segid 3A4 and resid 222 and name CB)	10.15	0.78	0.78
20	assign (segid 3A4 and resid 201 and name CB)	(segid 3A4 and resid 223 and name CA)	12.69	0.75	0.76
	assign (segid 3A4 and resid 201 and name CB)	(segid 3A4 and resid 223 and name CB)	13.36	0.74	0.73
	assign (segid 3A4 and resid 201 and name CB)	(segid 3A4 and resid 224 and name CA)	11.88	0.74	0.75
	assign (segid 3A4 and resid 201 and name CB)	(segid 3A4 and resid 224 and name CB)	11.09	0.59	0.59
	assign (segid 3A4 and resid 201 and name CB)	(segid 3A4 and resid 225 and name CA)	10.82	1.11	1.11
25	assign (segid 3A4 and resid 201 and name CB)	(segid 3A4 and resid 225 and name CB)	9.77	1.16	1.17
	assign (segid 3A4 and resid 201 and name CB)	(segid 3A4 and resid 226 and name CA)	14.05	1.20	1.20
	assign (segid 3A4 and resid 201 and name CB)	(segid 3A4 and resid 240 and name CA)	14.94	0.37	0.36
	assign (segid 3A4 and resid 201 and name CB)	(segid 3A4 and resid 240 and name CB)	15.90	0.39	0.38
	assign (segid 3A4 and resid 201 and name CB)	(segid 3A4 and resid 241 and name CA)	11.68	0.50	0.51
30	assign (segid 3A4 and resid 201 and name CB)	(segid 3A4 and resid 241 and name CB)	11.61	0.64	0.64
	assign (segid 3A4 and resid 201 and name CB)	(segid 3A4 and resid 242 and name CA)	12.87	0.59	0.58
	assign (segid 3A4 and resid 201 and name CB)	(segid 3A4 and resid 242 and name CB)	14.23	0.62	0.62
	assign (segid 3A4 and resid 201 and name CB)	(segid 3A4 and resid 243 and name CA)	13.80	0.44	0.43
	assign (segid 3A4 and resid 201 and name CB)	(segid 3A4 and resid 243 and name CB)	14.85	0.41	0.40
35	assign (segid 3A4 and resid 201 and name CB)	(segid 3A4 and resid 243 and name CB)	10.63	0.38	0.37
	assign (segid 3A4 and resid 201 and name CB)	(segid 3A4 and resid 244 and name CA)	9.98	0.41	0.41
	assign (segid 3A4 and resid 201 and name CB)	(segid 3A4 and resid 244 and name CB)	9.05	0.42	0.43
	assign (segid 3A4 and resid 201 and name CB)	(segid 3A4 and resid 245 and name CA)	9.26	0.44	0.43
	assign (segid 3A4 and resid 201 and name CB)	(segid 3A4 and resid 245 and name CB)	12.27	0.60	0.60
40	assign (segid 3A4 and resid 201 and name CB)	(segid 3A4 and resid 246 and name CA)	13.61	0.57	0.57
	assign (segid 3A4 and resid 201 and name CB)	(segid 3A4 and resid 246 and name CB)	12.35	0.45	0.45
	assign (segid 3A4 and resid 201 and name CB)	(segid 3A4 and resid 247 and name CA)	12.49	0.42	0.41
	assign (segid 3A4 and resid 201 and name CB)	(segid 3A4 and resid 247 and name CB)	9.21	0.54	0.54
	assign (segid 3A4 and resid 201 and name CB)	(segid 3A4 and resid 248 and name CA)	7.80	0.47	0.47
45	assign (segid 3A4 and resid 201 and name CB)	(segid 3A4 and resid 248 and name CB)	10.77	0.97	0.97
	assign (segid 3A4 and resid 201 and name CB)	(segid 3A4 and resid 249 and name CA)	13.98	0.86	0.87
	assign (segid 3A4 and resid 201 and name CB)	(segid 3A4 and resid 250 and name CA)	14.75	0.73	0.74
	assign (segid 3A4 and resid 201 and name CB)	(segid 3A4 and resid 250 and name CB)	13.23	0.74	0.74
	assign (segid 3A4 and resid 201 and name CB)	(segid 3A4 and resid 251 and name CA)	12.42	0.59	0.59
50	assign (segid 3A4 and resid 201 and name CB)	(segid 3A4 and resid 251 and name CB)	12.16	1.09	1.09
	assign (segid 3A4 and resid 201 and name CB)	(segid 3A4 and resid 252 and name CA)	11.03	1.17	1.16
	assign (segid 3A4 and resid 201 and name CB)	(segid 3A4 and resid 252 and name CB)	15.15	1.16	1.17
	assign (segid 3A4 and resid 201 and name CB)	(segid 3A4 and resid 253 and name CA)	17.54	0.99	1.00
	assign (segid 3A4 and resid 201 and name CB)	(segid 3A4 and resid 254 and name CA)	17.07	1.41	1.41
55	assign (segid 3A4 and resid 201 and name CB)	(segid 3A4 and resid 255 and name CA)	17.27	0.96	0.95
	assign (segid 3A4 and resid 201 and name CB)	(segid 3A4 and resid 256 and name CA)	2.44	0.01	0.02
	assign (segid 3A4 and resid 201 and name N)	(segid 3A4 and resid 201 and name C)	1.45	0.00	0.00
	assign (segid 3A4 and resid 201 and name N)	(segid 3A4 and resid 201 and name CB)	2.46	0.03	0.04
	assign (segid 3A4 and resid 201 and name N)	(segid 3A4 and resid 201 and name O)	3.48	0.04	0.03
60	assign (segid 3A4 and resid 201 and name N)	(segid 3A4 and resid 202 and name C)	4.73	0.05	0.06
	assign (segid 3A4 and resid 201 and name N)	(segid 3A4 and resid 202 and name CA)	4.24	0.05	0.04
	assign (segid 3A4 and resid 201 and name N)	(segid 3A4 and resid 202 and name CB)	4.98	0.04	0.05
	assign (segid 3A4 and resid 201 and name N)	(segid 3A4 and resid 202 and name CG1)	6.39	0.04	0.04
	assign (segid 3A4 and resid 201 and name N)	(segid 3A4 and resid 202 and name N)	2.81	0.04	0.05
65	assign (segid 3A4 and resid 201 and name N)	(segid 3A4 and resid 202 and name O)	5.80	0.03	0.04
	assign (segid 3A4 and resid 201 and name N)	(segid 3A4 and resid 203 and name C)	5.67	0.03	0.04
	assign (segid 3A4 and resid 201 and name N)	(segid 3A4 and resid 203 and name CA)	5.34	0.07	0.08
	assign (segid 3A4 and resid 201 and name N)	(segid 3A4 and resid 203 and name CB)	5.37	0.09	0.09
	assign (segid 3A4 and resid 201 and name N)	(segid 3A4 and resid 203 and name N)	4.34	0.09	0.10
70	assign (segid 3A4 and resid 201 and name N)	(segid 3A4 and resid 203 and name O)	6.87	0.04	0.03
	assign (segid 3A4 and resid 201 and name N)	(segid 3A4 and resid 204 and name C)	6.42	0.08	0.09
	assign (segid 3A4 and resid 201 and name N)	(segid 3A4 and resid 204 and name CA)	5.64	0.11	0.10
	assign (segid 3A4 and resid 201 and name N)	(segid 3A4 and resid 204 and name CB)	5.10	0.22	0.22
	assign (segid 3A4 and resid 201 and name N)	(segid 3A4 and resid 204 and name N)	4.87	0.06	0.05
75	assign (segid 3A4 and resid 201 and name N)	(segid 3A4 and resid 204 and name O)	7.59	0.08	0.09
	assign (segid 3A4 and resid 201 and name N)	(segid 3A4 and resid 205 and name CA)	7.11	0.12	0.11
	assign (segid 3A4 and resid 201 and name N)	(segid 3A4 and resid 205 and name CB)	6.80	0.16	0.17
	assign (segid 3A4 and resid 201 and name N)	(segid 3A4 and resid 205 and name N)	6.04	0.08	0.09
	assign (segid 3A4 and resid 201 and name N)	(segid 3A4 and resid 205 and name O)	3.30	0.06	0.06
80	assign (segid 3A4 and resid 201 and name O)	(segid 3A4 and resid 201 and name CB)	2.96	0.06	0.06
	assign (segid 3A4 and resid 201 and name O)	(segid 3A4 and resid 202 and name C)	2.78	0.03	0.03
	assign (segid 3A4 and resid 201 and name O)	(segid 3A4 and resid 202 and name CA)	4.28	0.02	0.02
	assign (segid 3A4 and resid 201 and name O)	(segid 3A4 and resid 202 and name CB)			

	assign (segid 3A4 and resid 201 and name O)	(segid 3A4 and resid 202 and name CG1)	5.25	0.05	0.05
	assign (segid 3A4 and resid 201 and name O)	(segid 3A4 and resid 202 and name N)	2.25	0.01	0.01
	assign (segid 3A4 and resid 201 and name O)	(segid 3A4 and resid 202 and name O)	3.43	0.07	0.06
	assign (segid 3A4 and resid 201 and name O)	(segid 3A4 and resid 203 and name C)	4.10	0.10	0.11
	assign (segid 3A4 and resid 201 and name O)	(segid 3A4 and resid 203 and name CA)	4.37	0.09	0.09
5	assign (segid 3A4 and resid 201 and name O)	(segid 3A4 and resid 203 and name CB)	5.31	0.08	0.09
	assign (segid 3A4 and resid 201 and name O)	(segid 3A4 and resid 203 and name N)	3.42	0.10	0.10
	assign (segid 3A4 and resid 201 and name O)	(segid 3A4 and resid 203 and name O)	4.98	0.11	0.11
	assign (segid 3A4 and resid 201 and name O)	(segid 3A4 and resid 204 and name C)	3.77	0.09	0.10
	assign (segid 3A4 and resid 201 and name O)	(segid 3A4 and resid 204 and name CA)	3.79	0.14	0.14
10	assign (segid 3A4 and resid 201 and name O)	(segid 3A4 and resid 204 and name CB)	3.71	0.25	0.25
	assign (segid 3A4 and resid 201 and name O)	(segid 3A4 and resid 204 and name N)	3.36	0.13	0.12
	assign (segid 3A4 and resid 201 and name O)	(segid 3A4 and resid 204 and name O)	4.91	0.09	0.09
	assign (segid 3A4 and resid 201 and name O)	(segid 3A4 and resid 205 and name C)	4.91	0.10	0.10
	assign (segid 3A4 and resid 201 and name O)	(segid 3A4 and resid 205 and name CA)	3.72	0.12	0.12
15	assign (segid 3A4 and resid 201 and name O)	(segid 3A4 and resid 205 and name CB)	3.35	0.16	0.16
	assign (segid 3A4 and resid 201 and name O)	(segid 3A4 and resid 205 and name N)	2.93	0.08	0.09
	assign (segid 3A4 and resid 201 and name O)	(segid 3A4 and resid 205 and name O)	5.97	0.11	0.11
	assign (segid 3A4 and resid 201 and name O)	(segid 3A4 and resid 206 and name C)	7.33	0.08	0.07
	assign (segid 3A4 and resid 201 and name O)	(segid 3A4 and resid 206 and name CA)	6.40	0.11	0.12
20	assign (segid 3A4 and resid 201 and name O)	(segid 3A4 and resid 206 and name CB)	6.70	0.17	0.16
	assign (segid 3A4 and resid 201 and name O)	(segid 3A4 and resid 206 and name N)	5.03	0.11	0.11
	assign (segid 3A4 and resid 201 and name O)	(segid 3A4 and resid 207 and name N)	7.01	0.06	0.06
	assign (segid 3A4 and resid 201 and name O)	(segid 3A4 and resid 221 and name CB)	6.06	0.43	0.44
	assign (segid 3A4 and resid 201 and name O)	(segid 3A4 and resid 202 and name CB)	2.53	0.03	0.04
25	assign (segid 3A4 and resid 202 and name C)	(segid 3A4 and resid 202 and name CG1)	2.90	0.06	0.07
	assign (segid 3A4 and resid 202 and name C)	(segid 3A4 and resid 202 and name O)	1.23	0.00	0.00
	assign (segid 3A4 and resid 202 and name C)	(segid 3A4 and resid 203 and name C)	3.04	0.04	0.03
	assign (segid 3A4 and resid 202 and name C)	(segid 3A4 and resid 203 and name CA)	2.45	0.03	0.03
	assign (segid 3A4 and resid 202 and name C)	(segid 3A4 and resid 203 and name CB)	3.72	0.03	0.03
30	assign (segid 3A4 and resid 202 and name C)	(segid 3A4 and resid 203 and name N)	1.33	0.00	0.00
	assign (segid 3A4 and resid 202 and name C)	(segid 3A4 and resid 203 and name O)	3.83	0.07	0.07
	assign (segid 3A4 and resid 202 and name C)	(segid 3A4 and resid 204 and name C)	4.55	0.04	0.04
	assign (segid 3A4 and resid 202 and name C)	(segid 3A4 and resid 204 and name CA)	4.50	0.07	0.07
	assign (segid 3A4 and resid 202 and name C)	(segid 3A4 and resid 204 and name CB)	5.27	0.16	0.16
35	assign (segid 3A4 and resid 202 and name C)	(segid 3A4 and resid 204 and name N)	3.35	0.06	0.06
	assign (segid 3A4 and resid 202 and name C)	(segid 3A4 and resid 204 and name O)	5.65	0.04	0.04
	assign (segid 3A4 and resid 202 and name C)	(segid 3A4 and resid 205 and name C)	4.77	0.07	0.07
	assign (segid 3A4 and resid 202 and name C)	(segid 3A4 and resid 205 and name CA)	4.42	0.10	0.11
	assign (segid 3A4 and resid 202 and name C)	(segid 3A4 and resid 205 and name CB)	4.25	0.20	0.20
40	assign (segid 3A4 and resid 202 and name C)	(segid 3A4 and resid 205 and name N)	3.72	0.08	0.07
	assign (segid 3A4 and resid 202 and name C)	(segid 3A4 and resid 205 and name O)	5.90	0.11	0.11
	assign (segid 3A4 and resid 202 and name C)	(segid 3A4 and resid 206 and name C)	6.26	0.06	0.05
	assign (segid 3A4 and resid 202 and name C)	(segid 3A4 and resid 206 and name CA)	5.08	0.05	0.06
	assign (segid 3A4 and resid 202 and name C)	(segid 3A4 and resid 206 and name CB)	4.74	0.11	0.11
45	assign (segid 3A4 and resid 202 and name C)	(segid 3A4 and resid 206 and name N)	4.16	0.02	0.02
	assign (segid 3A4 and resid 202 and name C)	(segid 3A4 and resid 206 and name O)	7.37	0.07	0.06
	assign (segid 3A4 and resid 202 and name C)	(segid 3A4 and resid 207 and name CA)	7.53	0.18	0.18
	assign (segid 3A4 and resid 202 and name C)	(segid 3A4 and resid 207 and name N)	6.22	0.14	0.15
	assign (segid 3A4 and resid 202 and name C)	(segid 3A4 and resid 221 and name CB)	7.08	0.40	0.41
50	assign (segid 3A4 and resid 202 and name C)	(segid 3A4 and resid 225 and name CB)	6.33	1.17	1.17
	assign (segid 3A4 and resid 202 and name CA)	(segid 3A4 and resid 202 and name C)	1.53	0.01	0.01
	assign (segid 3A4 and resid 202 and name CA)	(segid 3A4 and resid 202 and name CB)	1.55	0.01	0.01
	assign (segid 3A4 and resid 202 and name CA)	(segid 3A4 and resid 202 and name CG1)	2.53	0.03	0.04
	assign (segid 3A4 and resid 202 and name CA)	(segid 3A4 and resid 202 and name O)	2.41	0.03	0.02
55	assign (segid 3A4 and resid 202 and name CA)	(segid 3A4 and resid 203 and name C)	4.44	0.04	0.03
	assign (segid 3A4 and resid 202 and name CA)	(segid 3A4 and resid 203 and name CA)	3.81	0.02	0.03
	assign (segid 3A4 and resid 202 and name CA)	(segid 3A4 and resid 203 and name CB)	4.86	0.03	0.03
	assign (segid 3A4 and resid 202 and name CA)	(segid 3A4 and resid 203 and name N)	2.43	0.01	0.01
	assign (segid 3A4 and resid 202 and name CA)	(segid 3A4 and resid 203 and name O)	5.30	0.07	0.07
60	assign (segid 3A4 and resid 202 and name CA)	(segid 3A4 and resid 204 and name C)	5.50	0.02	0.03
	assign (segid 3A4 and resid 202 and name CA)	(segid 3A4 and resid 204 and name CA)	5.51	0.07	0.06
	assign (segid 3A4 and resid 202 and name CA)	(segid 3A4 and resid 204 and name CB)	5.95	0.18	0.18
	assign (segid 3A4 and resid 202 and name CA)	(segid 3A4 and resid 204 and name N)	4.46	0.06	0.05
	assign (segid 3A4 and resid 202 and name CA)	(segid 3A4 and resid 204 and name O)	6.64	0.02	0.02
65	assign (segid 3A4 and resid 202 and name CA)	(segid 3A4 and resid 205 and name C)	5.58	0.09	0.10
	assign (segid 3A4 and resid 202 and name CA)	(segid 3A4 and resid 205 and name CA)	5.02	0.10	0.10
	assign (segid 3A4 and resid 202 and name CA)	(segid 3A4 and resid 205 and name CB)	4.40	0.19	0.19
	assign (segid 3A4 and resid 202 and name CA)	(segid 3A4 and resid 205 and name N)	4.50	0.05	0.06
	assign (segid 3A4 and resid 202 and name CA)	(segid 3A4 and resid 205 and name O)	6.63	0.17	0.17
70	assign (segid 3A4 and resid 202 and name CA)	(segid 3A4 and resid 206 and name C)	7.51	0.05	0.05
	assign (segid 3A4 and resid 202 and name CA)	(segid 3A4 and resid 206 and name CA)	6.24	0.06	0.06
	assign (segid 3A4 and resid 202 and name CA)	(segid 3A4 and resid 206 and name CB)	6.00	0.09	0.10
	assign (segid 3A4 and resid 202 and name CA)	(segid 3A4 and resid 206 and name N)	5.24	0.03	0.02
	assign (segid 3A4 and resid 202 and name CA)	(segid 3A4 and resid 207 and name CA)	8.88	0.16	0.15
75	assign (segid 3A4 and resid 202 and name CA)	(segid 3A4 and resid 207 and name CB)	9.03	0.26	0.25
	assign (segid 3A4 and resid 202 and name CA)	(segid 3A4 and resid 207 and name N)	7.55	0.13	0.12
	assign (segid 3A4 and resid 202 and name CA)	(segid 3A4 and resid 219 and name CA)	11.49	0.31	0.31
	assign (segid 3A4 and resid 202 and name CA)	(segid 3A4 and resid 219 and name CB)	10.68	0.22	0.23
	assign (segid 3A4 and resid 202 and name CA)	(segid 3A4 and resid 220 and name CA)	10.68	0.46	0.46
80	assign (segid 3A4 and resid 202 and name CA)	(segid 3A4 and resid 220 and name CB)	11.15	0.53	0.54
	assign (segid 3A4 and resid 202 and name CA)	(segid 3A4 and resid 221 and name C)	6.93	0.58	0.58
	assign (segid 3A4 and resid 202 and name CA)	(segid 3A4 and resid 221 and name CA)	6.96	0.44	0.45

	assign (segid 3A4 and resid 202 and name CA)	(segid 3A4 and resid 221 and name CB)	6.01	0.41	0.40
	assign (segid 3A4 and resid 202 and name CA)	(segid 3A4 and resid 221 and name O)	6.69	0.72	0.71
	assign (segid 3A4 and resid 202 and name CA)	(segid 3A4 and resid 222 and name CA)	8.00	0.68	0.68
	assign (segid 3A4 and resid 202 and name CA)	(segid 3A4 and resid 222 and name CB)	8.96	0.62	0.62
	assign (segid 3A4 and resid 202 and name CA)	(segid 3A4 and resid 223 and name CA)	10.83	0.75	0.75
5	assign (segid 3A4 and resid 202 and name CA)	(segid 3A4 and resid 223 and name CB)	11.86	0.71	0.71
	assign (segid 3A4 and resid 202 and name CA)	(segid 3A4 and resid 224 and name CA)	9.38	0.75	0.75
	assign (segid 3A4 and resid 202 and name CA)	(segid 3A4 and resid 224 and name CB)	8.82	0.58	0.58
	assign (segid 3A4 and resid 202 and name CA)	(segid 3A4 and resid 225 and name CA)	7.33	1.18	1.18
	assign (segid 3A4 and resid 202 and name CA)	(segid 3A4 and resid 225 and name CB)	6.32	1.22	1.23
10	assign (segid 3A4 and resid 202 and name CA)	(segid 3A4 and resid 226 and name CA)	10.68	1.32	1.32
	assign (segid 3A4 and resid 202 and name CA)	(segid 3A4 and resid 240 and name CA)	11.12	0.47	0.46
	assign (segid 3A4 and resid 202 and name CA)	(segid 3A4 and resid 240 and name CB)	12.19	0.50	0.51
	assign (segid 3A4 and resid 202 and name CA)	(segid 3A4 and resid 241 and name CA)	8.00	0.64	0.64
	assign (segid 3A4 and resid 202 and name CA)	(segid 3A4 and resid 241 and name CB)	7.88	0.76	0.76
15	assign (segid 3A4 and resid 202 and name CA)	(segid 3A4 and resid 242 and name CA)	10.12	0.77	0.77
	assign (segid 3A4 and resid 202 and name CA)	(segid 3A4 and resid 242 and name CB)	11.49	0.79	0.79
	assign (segid 3A4 and resid 202 and name CA)	(segid 3A4 and resid 243 and name CA)	11.19	0.52	0.53
	assign (segid 3A4 and resid 202 and name CA)	(segid 3A4 and resid 243 and name CB)	12.01	0.52	0.52
	assign (segid 3A4 and resid 202 and name CA)	(segid 3A4 and resid 244 and name CA)	8.07	0.46	0.46
20	assign (segid 3A4 and resid 202 and name CA)	(segid 3A4 and resid 244 and name CB)	6.97	0.45	0.46
	assign (segid 3A4 and resid 202 and name CA)	(segid 3A4 and resid 245 and name CA)	7.64	0.64	0.63
	assign (segid 3A4 and resid 202 and name CA)	(segid 3A4 and resid 245 and name CB)	7.78	0.65	0.65
	assign (segid 3A4 and resid 202 and name CA)	(segid 3A4 and resid 246 and name CA)	11.32	0.68	0.68
	assign (segid 3A4 and resid 202 and name CA)	(segid 3A4 and resid 246 and name CB)	12.37	0.63	0.63
25	assign (segid 3A4 and resid 202 and name CA)	(segid 3A4 and resid 247 and name CA)	11.51	0.46	0.46
	assign (segid 3A4 and resid 202 and name CA)	(segid 3A4 and resid 247 and name CB)	11.28	0.35	0.34
	assign (segid 3A4 and resid 202 and name CA)	(segid 3A4 and resid 248 and name CA)	9.46	0.71	0.71
	assign (segid 3A4 and resid 202 and name CA)	(segid 3A4 and resid 248 and name CB)	8.04	0.77	0.76
	assign (segid 3A4 and resid 202 and name CA)	(segid 3A4 and resid 249 and name CA)	11.71	0.99	0.99
30	assign (segid 3A4 and resid 202 and name CA)	(segid 3A4 and resid 250 and name CA)	14.61	0.80	0.79
	assign (segid 3A4 and resid 202 and name CA)	(segid 3A4 and resid 250 and name CB)	14.96	0.64	0.65
	assign (segid 3A4 and resid 202 and name CA)	(segid 3A4 and resid 251 and name CA)	14.28	0.81	0.80
	assign (segid 3A4 and resid 202 and name CA)	(segid 3A4 and resid 251 and name CB)	13.31	0.74	0.74
35	assign (segid 3A4 and resid 202 and name CA)	(segid 3A4 and resid 252 and name CA)	14.28	1.09	1.10
	assign (segid 3A4 and resid 202 and name CA)	(segid 3A4 and resid 252 and name CB)	13.33	1.15	1.14
	assign (segid 3A4 and resid 202 and name CA)	(segid 3A4 and resid 253 and name CA)	17.14	1.02	1.02
	assign (segid 3A4 and resid 202 and name CB)	(segid 3A4 and resid 202 and name CG1)	1.52	0.02	0.02
	assign (segid 3A4 and resid 202 and name CB)	(segid 3A4 and resid 203 and name C)	5.46	0.05	0.05
40	assign (segid 3A4 and resid 202 and name CB)	(segid 3A4 and resid 203 and name CA)	4.49	0.04	0.05
	assign (segid 3A4 and resid 202 and name CB)	(segid 3A4 and resid 203 and name CB)	5.34	0.09	0.10
	assign (segid 3A4 and resid 202 and name CB)	(segid 3A4 and resid 203 and name N)	3.16	0.05	0.05
	assign (segid 3A4 and resid 202 and name CB)	(segid 3A4 and resid 203 and name O)	6.29	0.08	0.08
	assign (segid 3A4 and resid 202 and name CB)	(segid 3A4 and resid 204 and name C)	6.94	0.03	0.02
	assign (segid 3A4 and resid 202 and name CB)	(segid 3A4 and resid 204 and name CA)	6.88	0.08	0.07
45	assign (segid 3A4 and resid 202 and name CB)	(segid 3A4 and resid 204 and name CB)	7.38	0.18	0.18
	assign (segid 3A4 and resid 202 and name CB)	(segid 3A4 and resid 204 and name N)	5.70	0.08	0.07
	assign (segid 3A4 and resid 202 and name CB)	(segid 3A4 and resid 205 and name C)	6.77	0.13	0.13
	assign (segid 3A4 and resid 202 and name CB)	(segid 3A4 and resid 205 and name CA)	6.40	0.11	0.11
	assign (segid 3A4 and resid 202 and name CB)	(segid 3A4 and resid 205 and name CB)	5.72	0.20	0.20
50	assign (segid 3A4 and resid 202 and name CB)	(segid 3A4 and resid 205 and name N)	5.96	0.06	0.05
	assign (segid 3A4 and resid 202 and name CB)	(segid 3A4 and resid 206 and name CA)	7.05	0.08	0.09
	assign (segid 3A4 and resid 202 and name CB)	(segid 3A4 and resid 206 and name CB)	6.56	0.10	0.10
	assign (segid 3A4 and resid 202 and name CB)	(segid 3A4 and resid 206 and name N)	6.28	0.04	0.04
	assign (segid 3A4 and resid 202 and name CB)	(segid 3A4 and resid 207 and name CA)	9.94	0.16	0.17
55	assign (segid 3A4 and resid 202 and name CB)	(segid 3A4 and resid 207 and name CB)	10.13	0.25	0.25
	assign (segid 3A4 and resid 202 and name CB)	(segid 3A4 and resid 219 and name CA)	12.25	0.29	0.28
	assign (segid 3A4 and resid 202 and name CB)	(segid 3A4 and resid 219 and name CB)	11.53	0.23	0.24
	assign (segid 3A4 and resid 202 and name CB)	(segid 3A4 and resid 220 and name CA)	10.98	0.44	0.44
	assign (segid 3A4 and resid 202 and name CB)	(segid 3A4 and resid 220 and name CB)	11.33	0.56	0.55
60	assign (segid 3A4 and resid 202 and name CB)	(segid 3A4 and resid 221 and name CA)	7.28	0.40	0.40
	assign (segid 3A4 and resid 202 and name CB)	(segid 3A4 and resid 221 and name CB)	6.51	0.41	0.42
	assign (segid 3A4 and resid 202 and name CB)	(segid 3A4 and resid 221 and name O)	6.93	0.60	0.60
	assign (segid 3A4 and resid 202 and name CB)	(segid 3A4 and resid 222 and name CA)	8.67	0.55	0.55
	assign (segid 3A4 and resid 202 and name CB)	(segid 3A4 and resid 222 and name CB)	9.80	0.50	0.50
65	assign (segid 3A4 and resid 202 and name CB)	(segid 3A4 and resid 223 and name CA)	11.08	0.64	0.65
	assign (segid 3A4 and resid 202 and name CB)	(segid 3A4 and resid 223 and name CB)	12.08	0.62	0.61
	assign (segid 3A4 and resid 202 and name CB)	(segid 3A4 and resid 224 and name CA)	9.12	0.69	0.68
	assign (segid 3A4 and resid 202 and name CB)	(segid 3A4 and resid 224 and name CB)	8.43	0.55	0.56
	assign (segid 3A4 and resid 202 and name CB)	(segid 3A4 and resid 225 and name CA)	7.22	1.12	1.11
70	assign (segid 3A4 and resid 202 and name CB)	(segid 3A4 and resid 225 and name CB)	6.49	1.12	1.12
	assign (segid 3A4 and resid 202 and name CB)	(segid 3A4 and resid 226 and name CA)	10.76	1.23	1.23
	assign (segid 3A4 and resid 202 and name CB)	(segid 3A4 and resid 240 and name CA)	9.85	0.44	0.44
	assign (segid 3A4 and resid 202 and name CB)	(segid 3A4 and resid 240 and name CB)	10.86	0.48	0.49
	assign (segid 3A4 and resid 202 and name CB)	(segid 3A4 and resid 241 and name CA)	6.64	0.61	0.60
75	assign (segid 3A4 and resid 202 and name CB)	(segid 3A4 and resid 241 and name CB)	6.58	0.71	0.71
	assign (segid 3A4 and resid 202 and name CB)	(segid 3A4 and resid 241 and name O)	6.03	0.78	0.78
	assign (segid 3A4 and resid 202 and name CB)	(segid 3A4 and resid 242 and name CA)	8.61	0.79	0.79
	assign (segid 3A4 and resid 202 and name CB)	(segid 3A4 and resid 242 and name CB)	9.99	0.81	0.80
	assign (segid 3A4 and resid 202 and name CB)	(segid 3A4 and resid 243 and name CA)	9.78	0.57	0.57
80	assign (segid 3A4 and resid 202 and name CB)	(segid 3A4 and resid 243 and name CB)	10.65	0.54	0.54
	assign (segid 3A4 and resid 202 and name CB)	(segid 3A4 and resid 244 and name C)	6.52	0.62	0.61
	assign (segid 3A4 and resid 202 and name CB)	(segid 3A4 and resid 244 and name CA)	6.84	0.49	0.48

	assign (segid 3A4 and resid 202 and name O)	(segid 3A4 and resid 204 and name CB)	5.43	0.15	0.14
	assign (segid 3A4 and resid 202 and name O)	(segid 3A4 and resid 204 and name N)	3.51	0.07	0.06
	assign (segid 3A4 and resid 202 and name O)	(segid 3A4 and resid 204 and name O)	5.08	0.07	0.07
	assign (segid 3A4 and resid 202 and name O)	(segid 3A4 and resid 205 and name C)	3.72	0.09	0.08
5	assign (segid 3A4 and resid 202 and name O)	(segid 3A4 and resid 205 and name CA)	3.67	0.14	0.14
	assign (segid 3A4 and resid 202 and name O)	(segid 3A4 and resid 205 and name CB)	3.64	0.24	0.24
	assign (segid 3A4 and resid 202 and name O)	(segid 3A4 and resid 205 and name N)	3.23	0.12	0.11
	assign (segid 3A4 and resid 202 and name O)	(segid 3A4 and resid 205 and name O)	4.81	0.12	0.12
	assign (segid 3A4 and resid 202 and name O)	(segid 3A4 and resid 206 and name C)	5.14	0.05	0.06
10	assign (segid 3A4 and resid 202 and name O)	(segid 3A4 and resid 206 and name CA)	3.90	0.06	0.06
	assign (segid 3A4 and resid 202 and name O)	(segid 3A4 and resid 206 and name CB)	3.66	0.13	0.12
	assign (segid 3A4 and resid 202 and name O)	(segid 3A4 and resid 206 and name N)	3.02	0.03	0.04
	assign (segid 3A4 and resid 202 and name O)	(segid 3A4 and resid 206 and name O)	6.22	0.06	0.06
	assign (segid 3A4 and resid 202 and name O)	(segid 3A4 and resid 207 and name C)	7.40	0.16	0.17
15	assign (segid 3A4 and resid 202 and name O)	(segid 3A4 and resid 207 and name CA)	6.63	0.17	0.16
	assign (segid 3A4 and resid 202 and name O)	(segid 3A4 and resid 207 and name CB)	6.93	0.24	0.24
	assign (segid 3A4 and resid 202 and name O)	(segid 3A4 and resid 207 and name N)	5.26	0.14	0.13
	assign (segid 3A4 and resid 202 and name O)	(segid 3A4 and resid 221 and name CB)	7.04	0.41	0.41
	assign (segid 3A4 and resid 202 and name O)	(segid 3A4 and resid 221 and name O)	6.86	0.59	0.60
20	assign (segid 3A4 and resid 202 and name O)	(segid 3A4 and resid 225 and name CB)	5.49	1.10	1.10
	assign (segid 3A4 and resid 203 and name C)	(segid 3A4 and resid 203 and name CB)	2.49	0.02	0.02
	assign (segid 3A4 and resid 203 and name C)	(segid 3A4 and resid 203 and name O)	1.23	0.00	0.00
	assign (segid 3A4 and resid 203 and name C)	(segid 3A4 and resid 204 and name C)	3.02	0.02	0.02
25	assign (segid 3A4 and resid 203 and name C)	(segid 3A4 and resid 204 and name CA)	2.43	0.03	0.04
	assign (segid 3A4 and resid 203 and name C)	(segid 3A4 and resid 204 and name CB)	3.72	0.05	0.04
	assign (segid 3A4 and resid 203 and name C)	(segid 3A4 and resid 204 and name N)	1.32	0.01	0.02
	assign (segid 3A4 and resid 203 and name C)	(segid 3A4 and resid 204 and name O)	3.93	0.05	0.05
	assign (segid 3A4 and resid 203 and name C)	(segid 3A4 and resid 205 and name C)	4.58	0.07	0.07
30	assign (segid 3A4 and resid 203 and name C)	(segid 3A4 and resid 205 and name CA)	4.40	0.10	0.10
	assign (segid 3A4 and resid 203 and name C)	(segid 3A4 and resid 205 and name CB)	5.18	0.15	0.15
	assign (segid 3A4 and resid 203 and name C)	(segid 3A4 and resid 205 and name N)	3.19	0.10	0.09
	assign (segid 3A4 and resid 203 and name C)	(segid 3A4 and resid 205 and name O)	5.75	0.07	0.07
	assign (segid 3A4 and resid 203 and name C)	(segid 3A4 and resid 206 and name C)	5.05	0.05	0.05
35	assign (segid 3A4 and resid 203 and name C)	(segid 3A4 and resid 206 and name CA)	4.58	0.10	0.10
	assign (segid 3A4 and resid 203 and name C)	(segid 3A4 and resid 206 and name CB)	4.32	0.17	0.17
	assign (segid 3A4 and resid 203 and name C)	(segid 3A4 and resid 206 and name N)	3.79	0.10	0.09
	assign (segid 3A4 and resid 203 and name C)	(segid 3A4 and resid 206 and name O)	6.22	0.10	0.10
	assign (segid 3A4 and resid 203 and name C)	(segid 3A4 and resid 207 and name C)	6.38	0.23	0.23
40	assign (segid 3A4 and resid 203 and name C)	(segid 3A4 and resid 207 and name CA)	5.41	0.22	0.22
	assign (segid 3A4 and resid 203 and name C)	(segid 3A4 and resid 207 and name CB)	5.06	0.32	0.32
	assign (segid 3A4 and resid 203 and name C)	(segid 3A4 and resid 207 and name N)	4.45	0.13	0.14
	assign (segid 3A4 and resid 203 and name C)	(segid 3A4 and resid 207 and name O)	7.54	0.18	0.18
	assign (segid 3A4 and resid 203 and name CA)	(segid 3A4 and resid 203 and name C)	1.53	0.02	0.01
45	assign (segid 3A4 and resid 203 and name CA)	(segid 3A4 and resid 203 and name CB)	1.53	0.02	0.01
	assign (segid 3A4 and resid 203 and name CA)	(segid 3A4 and resid 203 and name O)	2.40	0.01	0.02
	assign (segid 3A4 and resid 203 and name CA)	(segid 3A4 and resid 204 and name C)	4.41	0.03	0.02
	assign (segid 3A4 and resid 203 and name CA)	(segid 3A4 and resid 204 and name CA)	3.79	0.03	0.04
	assign (segid 3A4 and resid 203 and name CA)	(segid 3A4 and resid 204 and name CB)	4.84	0.08	0.09
50	assign (segid 3A4 and resid 203 and name CA)	(segid 3A4 and resid 204 and name N)	2.41	0.04	0.04
	assign (segid 3A4 and resid 203 and name CA)	(segid 3A4 and resid 204 and name O)	5.39	0.06	0.06
	assign (segid 3A4 and resid 203 and name CA)	(segid 3A4 and resid 205 and name C)	5.50	0.06	0.07
	assign (segid 3A4 and resid 203 and name CA)	(segid 3A4 and resid 205 and name CA)	5.37	0.10	0.11
	assign (segid 3A4 and resid 203 and name CA)	(segid 3A4 and resid 205 and name CB)	5.83	0.19	0.20
55	assign (segid 3A4 and resid 203 and name CA)	(segid 3A4 and resid 205 and name N)	4.27	0.09	0.09
	assign (segid 3A4 and resid 203 and name CA)	(segid 3A4 and resid 205 and name O)	6.67	0.06	0.06
	assign (segid 3A4 and resid 203 and name CA)	(segid 3A4 and resid 206 and name C)	5.94	0.06	0.06
	assign (segid 3A4 and resid 203 and name CA)	(segid 3A4 and resid 206 and name CA)	5.22	0.07	0.06
	assign (segid 3A4 and resid 203 and name CA)	(segid 3A4 and resid 206 and name CB)	4.58	0.13	0.12
60	assign (segid 3A4 and resid 203 and name CA)	(segid 3A4 and resid 206 and name N)	4.58	0.06	0.06
	assign (segid 3A4 and resid 203 and name CA)	(segid 3A4 and resid 206 and name O)	7.06	0.13	0.13
	assign (segid 3A4 and resid 203 and name CA)	(segid 3A4 and resid 207 and name CA)	6.63	0.23	0.23
	assign (segid 3A4 and resid 203 and name CA)	(segid 3A4 and resid 207 and name CB)	6.34	0.33	0.34
	assign (segid 3A4 and resid 203 and name CA)	(segid 3A4 and resid 207 and name N)	5.57	0.16	0.16
65	assign (segid 3A4 and resid 203 and name CA)	(segid 3A4 and resid 219 and name CA)	14.26	0.43	0.43
	assign (segid 3A4 and resid 203 and name CA)	(segid 3A4 and resid 219 and name CB)	13.44	0.37	0.36
	assign (segid 3A4 and resid 203 and name CA)	(segid 3A4 and resid 220 and name CA)	13.99	0.45	0.46
	assign (segid 3A4 and resid 203 and name CA)	(segid 3A4 and resid 220 and name CB)	14.65	0.51	0.51
	assign (segid 3A4 and resid 203 and name CA)	(segid 3A4 and resid 221 and name CA)	10.29	0.43	0.44
70	assign (segid 3A4 and resid 203 and name CA)	(segid 3A4 and resid 221 and name CB)	9.42	0.42	0.43
	assign (segid 3A4 and resid 203 and name CA)	(segid 3A4 and resid 222 and name CA)	10.28	0.74	0.74
	assign (segid 3A4 and resid 203 and name CA)	(segid 3A4 and resid 222 and name CB)	10.98	0.73	0.74
	assign (segid 3A4 and resid 203 and name CA)	(segid 3A4 and resid 223 and name CA)	13.33	0.78	0.79
	assign (segid 3A4 and resid 203 and name CA)	(segid 3A4 and resid 223 and name CB)	14.57	0.74	0.74
	assign (segid 3A4 and resid 203 and name CA)	(segid 3A4 and resid 224 and name CA)	12.16	0.65	0.66
75	assign (segid 3A4 and resid 203 and name CA)	(segid 3A4 and resid 224 and name CB)	11.89	0.50	0.50
	assign (segid 3A4 and resid 203 and name CA)	(segid 3A4 and resid 225 and name CA)	9.25	1.01	1.01
	assign (segid 3A4 and resid 203 and name CA)	(segid 3A4 and resid 225 and name CB)	8.10	1.02	1.02
	assign (segid 3A4 and resid 203 and name CA)	(segid 3A4 and resid 226 and name CA)	11.91	1.40	1.39
80	assign (segid 3A4 and resid 203 and name CA)	(segid 3A4 and resid 240 and name CA)	12.23	0.71	0.71
	assign (segid 3A4 and resid 203 and name CA)	(segid 3A4 and resid 240 and name CB)	13.22	0.80	0.81
	assign (segid 3A4 and resid 203 and name CA)	(segid 3A4 and resid 241 and name CA)	9.10	0.86	0.87
	assign (segid 3A4 and resid 203 and name CA)	(segid 3A4 and resid 241 and name CB)	8.40	1.01	1.02
	assign (segid 3A4 and resid 203 and name CA)	(segid 3A4 and resid 242 and name CA)	11.69	1.02	1.02

	assign (segid 3A4 and resid 203 and name CA)	(segid 3A4 and resid 242 and name CB)	12.82	1.10	1.10
	assign (segid 3A4 and resid 203 and name CA)	(segid 3A4 and resid 243 and name CA)	13.53	0.70	0.70
	assign (segid 3A4 and resid 203 and name CA)	(segid 3A4 and resid 243 and name CB)	14.26	0.70	0.70
	assign (segid 3A4 and resid 203 and name CA)	(segid 3A4 and resid 244 and name CA)	10.93	0.55	0.56
5	assign (segid 3A4 and resid 203 and name CA)	(segid 3A4 and resid 244 and name CB)	9.69	0.50	0.50
	assign (segid 3A4 and resid 203 and name CA)	(segid 3A4 and resid 245 and name CA)	10.54	0.74	0.75
	assign (segid 3A4 and resid 203 and name CA)	(segid 3A4 and resid 245 and name CB)	10.25	0.81	0.81
	assign (segid 3A4 and resid 203 and name CA)	(segid 3A4 and resid 246 and name CA)	14.30	0.78	0.77
	assign (segid 3A4 and resid 203 and name CA)	(segid 3A4 and resid 246 and name CB)	15.17	0.75	0.75
10	assign (segid 3A4 and resid 203 and name CA)	(segid 3A4 and resid 247 and name CA)	14.97	0.51	0.50
	assign (segid 3A4 and resid 203 and name CA)	(segid 3A4 and resid 247 and name CB)	14.71	0.38	0.38
	assign (segid 3A4 and resid 203 and name CA)	(segid 3A4 and resid 248 and name CA)	13.15	0.70	0.70
	assign (segid 3A4 and resid 203 and name CA)	(segid 3A4 and resid 248 and name CB)	11.72	0.75	0.75
	assign (segid 3A4 and resid 203 and name CA)	(segid 3A4 and resid 249 and name CA)	15.11	1.00	0.99
	assign (segid 3A4 and resid 203 and name CA)	(segid 3A4 and resid 250 and name CA)	18.16	0.79	0.80
15	assign (segid 3A4 and resid 203 and name CA)	(segid 3A4 and resid 250 and name CB)	18.50	0.65	0.65
	assign (segid 3A4 and resid 203 and name CA)	(segid 3A4 and resid 251 and name CA)	18.04	0.80	0.80
	assign (segid 3A4 and resid 203 and name CA)	(segid 3A4 and resid 251 and name CB)	17.10	0.74	0.75
	assign (segid 3A4 and resid 203 and name CA)	(segid 3A4 and resid 252 and name CA)	17.88	1.08	1.08
	assign (segid 3A4 and resid 203 and name CA)	(segid 3A4 and resid 252 and name CB)	16.82	1.13	1.14
20	assign (segid 3A4 and resid 203 and name CA)	(segid 3A4 and resid 204 and name C)	5.38	0.04	0.05
	assign (segid 3A4 and resid 203 and name CB)	(segid 3A4 and resid 204 and name CA)	4.40	0.06	0.07
	assign (segid 3A4 and resid 203 and name CB)	(segid 3A4 and resid 204 and name CB)	5.25	0.13	0.12
	assign (segid 3A4 and resid 203 and name CB)	(segid 3A4 and resid 204 and name N)	3.07	0.06	0.06
25	assign (segid 3A4 and resid 203 and name CB)	(segid 3A4 and resid 204 and name O)	6.33	0.07	0.07
	assign (segid 3A4 and resid 203 and name CB)	(segid 3A4 and resid 205 and name C)	6.92	0.07	0.07
	assign (segid 3A4 and resid 203 and name CB)	(segid 3A4 and resid 205 and name CA)	6.72	0.11	0.10
	assign (segid 3A4 and resid 203 and name CB)	(segid 3A4 and resid 205 and name CB)	7.21	0.17	0.18
	assign (segid 3A4 and resid 203 and name CB)	(segid 3A4 and resid 205 and name N)	5.49	0.10	0.09
30	assign (segid 3A4 and resid 203 and name CB)	(segid 3A4 and resid 206 and name C)	7.12	0.07	0.06
	assign (segid 3A4 and resid 203 and name CB)	(segid 3A4 and resid 206 and name CA)	6.57	0.09	0.08
	assign (segid 3A4 and resid 203 and name CB)	(segid 3A4 and resid 206 and name CB)	5.83	0.14	0.15
	assign (segid 3A4 and resid 203 and name CB)	(segid 3A4 and resid 206 and name N)	6.00	0.07	0.07
	assign (segid 3A4 and resid 203 and name CB)	(segid 3A4 and resid 207 and name CA)	7.47	0.25	0.24
35	assign (segid 3A4 and resid 203 and name CB)	(segid 3A4 and resid 207 and name CB)	6.91	0.35	0.35
	assign (segid 3A4 and resid 203 and name CB)	(segid 3A4 and resid 207 and name N)	6.61	0.16	0.16
	assign (segid 3A4 and resid 203 and name CB)	(segid 3A4 and resid 219 and name CA)	15.57	0.42	0.41
	assign (segid 3A4 and resid 203 and name CB)	(segid 3A4 and resid 219 and name CB)	14.67	0.35	0.35
	assign (segid 3A4 and resid 203 and name CB)	(segid 3A4 and resid 220 and name CA)	15.30	0.43	0.43
40	assign (segid 3A4 and resid 203 and name CB)	(segid 3A4 and resid 220 and name CB)	15.88	0.49	0.50
	assign (segid 3A4 and resid 203 and name CB)	(segid 3A4 and resid 221 and name CA)	11.59	0.43	0.42
	assign (segid 3A4 and resid 203 and name CB)	(segid 3A4 and resid 221 and name CB)	10.63	0.40	0.41
	assign (segid 3A4 and resid 203 and name CB)	(segid 3A4 and resid 222 and name CA)	11.75	0.74	0.73
	assign (segid 3A4 and resid 203 and name CB)	(segid 3A4 and resid 222 and name CB)	12.44	0.75	0.75
45	assign (segid 3A4 and resid 203 and name CB)	(segid 3A4 and resid 223 and name CA)	14.81	0.76	0.76
	assign (segid 3A4 and resid 203 and name CB)	(segid 3A4 and resid 223 and name CB)	16.03	0.71	0.71
	assign (segid 3A4 and resid 203 and name CB)	(segid 3A4 and resid 224 and name CA)	13.53	0.63	0.64
	assign (segid 3A4 and resid 203 and name CB)	(segid 3A4 and resid 224 and name CB)	13.19	0.50	0.49
	assign (segid 3A4 and resid 203 and name CB)	(segid 3A4 and resid 225 and name CA)	10.66	0.99	0.99
50	assign (segid 3A4 and resid 203 and name CB)	(segid 3A4 and resid 225 and name CB)	9.56	1.01	1.00
	assign (segid 3A4 and resid 203 and name CB)	(segid 3A4 and resid 226 and name CA)	13.35	1.37	1.37
	assign (segid 3A4 and resid 203 and name CB)	(segid 3A4 and resid 240 and name CA)	12.86	0.68	0.67
	assign (segid 3A4 and resid 203 and name CB)	(segid 3A4 and resid 240 and name CB)	13.72	0.78	0.79
	assign (segid 3A4 and resid 203 and name CB)	(segid 3A4 and resid 241 and name CA)	9.59	0.78	0.78
55	assign (segid 3A4 and resid 203 and name CB)	(segid 3A4 and resid 241 and name CB)	8.72	0.93	0.92
	assign (segid 3A4 and resid 203 and name CB)	(segid 3A4 and resid 242 and name CA)	11.93	1.02	1.01
	assign (segid 3A4 and resid 203 and name CB)	(segid 3A4 and resid 242 and name CB)	12.95	1.11	1.11
	assign (segid 3A4 and resid 203 and name CB)	(segid 3A4 and resid 243 and name CA)	14.11	0.67	0.67
	assign (segid 3A4 and resid 203 and name CB)	(segid 3A4 and resid 243 and name CB)	14.93	0.66	0.66
60	assign (segid 3A4 and resid 203 and name CB)	(segid 3A4 and resid 244 and name CA)	11.76	0.47	0.48
	assign (segid 3A4 and resid 203 and name CB)	(segid 3A4 and resid 244 and name CB)	10.59	0.41	0.42
	assign (segid 3A4 and resid 203 and name CB)	(segid 3A4 and resid 245 and name CA)	11.00	0.69	0.69
	assign (segid 3A4 and resid 203 and name CB)	(segid 3A4 and resid 245 and name CB)	10.52	0.77	0.76
	assign (segid 3A4 and resid 203 and name CB)	(segid 3A4 and resid 246 and name CA)	14.72	0.73	0.74
65	assign (segid 3A4 and resid 203 and name CB)	(segid 3A4 and resid 246 and name CB)	15.57	0.72	0.73
	assign (segid 3A4 and resid 203 and name CB)	(segid 3A4 and resid 247 and name CA)	15.72	0.45	0.46
	assign (segid 3A4 and resid 203 and name CB)	(segid 3A4 and resid 247 and name CB)	15.58	0.33	0.33
	assign (segid 3A4 and resid 203 and name CB)	(segid 3A4 and resid 248 and name CA)	13.89	0.61	0.62
	assign (segid 3A4 and resid 203 and name CB)	(segid 3A4 and resid 248 and name CB)	12.45	0.65	0.65
70	assign (segid 3A4 and resid 203 and name CB)	(segid 3A4 and resid 249 and name CA)	15.53	0.95	0.94
	assign (segid 3A4 and resid 203 and name CB)	(segid 3A4 and resid 250 and name CA)	18.73	0.76	0.77
	assign (segid 3A4 and resid 203 and name CB)	(segid 3A4 and resid 251 and name CA)	18.81	0.73	0.73
	assign (segid 3A4 and resid 203 and name CB)	(segid 3A4 and resid 251 and name CB)	17.96	0.66	0.66
	assign (segid 3A4 and resid 203 and name CB)	(segid 3A4 and resid 252 and name CA)	18.45	1.00	1.00
75	assign (segid 3A4 and resid 203 and name CB)	(segid 3A4 and resid 252 and name CB)	17.31	1.05	1.05
	assign (segid 3A4 and resid 203 and name N)	(segid 3A4 and resid 203 and name C)	2.46	0.02	0.03
	assign (segid 3A4 and resid 203 and name N)	(segid 3A4 and resid 203 and name CA)	1.46	0.01	0.01
	assign (segid 3A4 and resid 203 and name N)	(segid 3A4 and resid 203 and name CB)	2.46	0.03	0.03
	assign (segid 3A4 and resid 203 and name N)	(segid 3A4 and resid 203 and name O)	3.48	0.03	0.03
80	assign (segid 3A4 and resid 203 and name N)	(segid 3A4 and resid 204 and name C)	4.67	0.03	0.04
	assign (segid 3A4 and resid 203 and name N)	(segid 3A4 and resid 204 and name CA)	4.21	0.07	0.08
	assign (segid 3A4 and resid 203 and name N)	(segid 3A4 and resid 204 and name CB)	4.97	0.15	0.15
	assign (segid 3A4 and resid 203 and name N)	(segid 3A4 and resid 204 and name N)	2.82	0.07	0.08

	assign (segid 3A4 and resid 203 and name N)	(segid 3A4 and resid 204 and name O)	5.81	0.05	0.05
	assign (segid 3A4 and resid 203 and name N)	(segid 3A4 and resid 205 and name C)	5.55	0.04	0.05
	assign (segid 3A4 and resid 203 and name N)	(segid 3A4 and resid 205 and name CA)	5.19	0.08	0.09
	assign (segid 3A4 and resid 203 and name N)	(segid 3A4 and resid 205 and name CB)	5.28	0.18	0.18
	assign (segid 3A4 and resid 203 and name N)	(segid 3A4 and resid 205 and name N)	4.18	0.06	0.07
5	assign (segid 3A4 and resid 203 and name N)	(segid 3A4 and resid 205 and name O)	6.73	0.05	0.06
	assign (segid 3A4 and resid 203 and name N)	(segid 3A4 and resid 206 and name C)	6.64	0.07	0.07
	assign (segid 3A4 and resid 203 and name N)	(segid 3A4 and resid 206 and name CA)	5.66	0.05	0.06
	assign (segid 3A4 and resid 203 and name N)	(segid 3A4 and resid 206 and name CB)	5.15	0.10	0.10
	assign (segid 3A4 and resid 203 and name N)	(segid 3A4 and resid 206 and name N)	4.82	0.03	0.03
10	assign (segid 3A4 and resid 203 and name N)	(segid 3A4 and resid 206 and name O)	7.78	0.10	0.10
	assign (segid 3A4 and resid 203 and name N)	(segid 3A4 and resid 207 and name N)	6.41	0.15	0.14
	assign (segid 3A4 and resid 203 and name N)	(segid 3A4 and resid 203 and name CB)	3.32	0.03	0.04
	assign (segid 3A4 and resid 203 and name O)	(segid 3A4 and resid 204 and name C)	2.99	0.04	0.04
	assign (segid 3A4 and resid 203 and name O)	(segid 3A4 and resid 204 and name CA)	2.77	0.05	0.05
15	assign (segid 3A4 and resid 203 and name O)	(segid 3A4 and resid 204 and name CB)	4.26	0.04	0.04
	assign (segid 3A4 and resid 203 and name O)	(segid 3A4 and resid 204 and name N)	2.24	0.01	0.01
	assign (segid 3A4 and resid 203 and name O)	(segid 3A4 and resid 204 and name O)	3.56	0.06	0.07
	assign (segid 3A4 and resid 203 and name O)	(segid 3A4 and resid 205 and name C)	4.16	0.14	0.13
	assign (segid 3A4 and resid 203 and name O)	(segid 3A4 and resid 205 and name CA)	4.33	0.14	0.13
20	assign (segid 3A4 and resid 203 and name O)	(segid 3A4 and resid 205 and name CB)	5.34	0.19	0.20
	assign (segid 3A4 and resid 203 and name O)	(segid 3A4 and resid 205 and name N)	3.33	0.13	0.13
	assign (segid 3A4 and resid 203 and name O)	(segid 3A4 and resid 205 and name O)	5.21	0.14	0.14
	assign (segid 3A4 and resid 203 and name O)	(segid 3A4 and resid 206 and name C)	3.99	0.05	0.05
	assign (segid 3A4 and resid 203 and name O)	(segid 3A4 and resid 206 and name CA)	3.76	0.14	0.15
25	assign (segid 3A4 and resid 203 and name O)	(segid 3A4 and resid 206 and name CB)	3.56	0.21	0.21
	assign (segid 3A4 and resid 203 and name O)	(segid 3A4 and resid 206 and name N)	3.23	0.17	0.16
	assign (segid 3A4 and resid 203 and name O)	(segid 3A4 and resid 206 and name O)	5.13	0.10	0.10
	assign (segid 3A4 and resid 203 and name O)	(segid 3A4 and resid 207 and name C)	5.34	0.23	0.24
	assign (segid 3A4 and resid 203 and name O)	(segid 3A4 and resid 207 and name CA)	4.26	0.22	0.23
30	assign (segid 3A4 and resid 203 and name O)	(segid 3A4 and resid 207 and name CB)	3.99	0.33	0.34
	assign (segid 3A4 and resid 203 and name O)	(segid 3A4 and resid 207 and name N)	3.33	0.13	0.14
	assign (segid 3A4 and resid 203 and name O)	(segid 3A4 and resid 207 and name O)	6.48	0.21	0.20
	assign (segid 3A4 and resid 203 and name O)	(segid 3A4 and resid 204 and name CB)	2.48	0.02	0.02
35	assign (segid 3A4 and resid 204 and name C)	(segid 3A4 and resid 204 and name O)	1.23	0.00	0.00
	assign (segid 3A4 and resid 204 and name C)	(segid 3A4 and resid 205 and name C)	3.15	0.06	0.06
	assign (segid 3A4 and resid 204 and name C)	(segid 3A4 and resid 205 and name CA)	2.43	0.01	0.02
	assign (segid 3A4 and resid 204 and name C)	(segid 3A4 and resid 205 and name CB)	3.67	0.03	0.02
	assign (segid 3A4 and resid 204 and name C)	(segid 3A4 and resid 205 and name N)	1.33	0.01	0.00
40	assign (segid 3A4 and resid 204 and name C)	(segid 3A4 and resid 205 and name O)	4.14	0.12	0.11
	assign (segid 3A4 and resid 204 and name C)	(segid 3A4 and resid 206 and name C)	4.67	0.05	0.05
	assign (segid 3A4 and resid 204 and name C)	(segid 3A4 and resid 206 and name CA)	4.51	0.10	0.10
	assign (segid 3A4 and resid 204 and name C)	(segid 3A4 and resid 206 and name CB)	5.21	0.14	0.15
	assign (segid 3A4 and resid 204 and name C)	(segid 3A4 and resid 206 and name N)	3.28	0.10	0.09
	assign (segid 3A4 and resid 204 and name C)	(segid 3A4 and resid 206 and name O)	5.80	0.05	0.04
45	assign (segid 3A4 and resid 204 and name C)	(segid 3A4 and resid 207 and name C)	4.89	0.18	0.19
	assign (segid 3A4 and resid 204 and name C)	(segid 3A4 and resid 207 and name CA)	4.65	0.11	0.10
	assign (segid 3A4 and resid 204 and name C)	(segid 3A4 and resid 207 and name CB)	4.54	0.19	0.19
	assign (segid 3A4 and resid 204 and name C)	(segid 3A4 and resid 207 and name N)	3.90	0.06	0.06
	assign (segid 3A4 and resid 204 and name C)	(segid 3A4 and resid 207 and name O)	6.04	0.11	0.11
50	assign (segid 3A4 and resid 204 and name C)	(segid 3A4 and resid 204 and name CB)	1.52	0.00	0.00
	assign (segid 3A4 and resid 204 and name CA)	(segid 3A4 and resid 204 and name O)	1.53	0.01	0.01
	assign (segid 3A4 and resid 204 and name CA)	(segid 3A4 and resid 205 and name C)	2.39	0.01	0.01
	assign (segid 3A4 and resid 204 and name CA)	(segid 3A4 and resid 205 and name CA)	4.52	0.05	0.05
	assign (segid 3A4 and resid 204 and name CA)	(segid 3A4 and resid 205 and name CB)	3.80	0.01	0.01
55	assign (segid 3A4 and resid 204 and name CA)	(segid 3A4 and resid 205 and name N)	4.82	0.03	0.02
	assign (segid 3A4 and resid 204 and name CA)	(segid 3A4 and resid 205 and name O)	2.43	0.01	0.02
	assign (segid 3A4 and resid 204 and name CA)	(segid 3A4 and resid 206 and name C)	5.58	0.11	0.10
	assign (segid 3A4 and resid 204 and name CA)	(segid 3A4 and resid 206 and name CA)	5.62	0.07	0.06
	assign (segid 3A4 and resid 204 and name CA)	(segid 3A4 and resid 206 and name CB)	5.47	0.13	0.13
60	assign (segid 3A4 and resid 204 and name CA)	(segid 3A4 and resid 206 and name N)	5.84	0.19	0.19
	assign (segid 3A4 and resid 204 and name CA)	(segid 3A4 and resid 206 and name O)	4.35	0.11	0.12
	assign (segid 3A4 and resid 204 and name CA)	(segid 3A4 and resid 207 and name C)	6.77	0.05	0.05
	assign (segid 3A4 and resid 204 and name CA)	(segid 3A4 and resid 207 and name CA)	5.80	0.18	0.18
65	assign (segid 3A4 and resid 204 and name CA)	(segid 3A4 and resid 207 and name CB)	5.33	0.12	0.12
	assign (segid 3A4 and resid 204 and name CA)	(segid 3A4 and resid 207 and name N)	4.80	0.23	0.24
	assign (segid 3A4 and resid 204 and name CA)	(segid 3A4 and resid 207 and name O)	4.71	0.05	0.05
	assign (segid 3A4 and resid 204 and name CA)	(segid 3A4 and resid 219 and name CA)	6.93	0.09	0.10
	assign (segid 3A4 and resid 204 and name CA)	(segid 3A4 and resid 219 and name CB)	12.94	0.67	0.67
70	assign (segid 3A4 and resid 204 and name CA)	(segid 3A4 and resid 220 and name CA)	11.96	0.61	0.60
	assign (segid 3A4 and resid 204 and name CA)	(segid 3A4 and resid 220 and name CB)	13.68	0.63	0.64
	assign (segid 3A4 and resid 204 and name CA)	(segid 3A4 and resid 221 and name CA)	14.49	0.59	0.60
	assign (segid 3A4 and resid 204 and name CA)	(segid 3A4 and resid 221 and name CB)	10.36	0.61	0.60
	assign (segid 3A4 and resid 204 and name CA)	(segid 3A4 and resid 221 and name N)	9.32	0.51	0.51
75	assign (segid 3A4 and resid 204 and name CA)	(segid 3A4 and resid 222 and name CA)	9.76	0.99	0.99
	assign (segid 3A4 and resid 204 and name CA)	(segid 3A4 and resid 222 and name CB)	9.95	1.01	1.01
	assign (segid 3A4 and resid 204 and name CA)	(segid 3A4 and resid 223 and name CA)	13.37	1.01	1.00
	assign (segid 3A4 and resid 204 and name CA)	(segid 3A4 and resid 223 and name CB)	14.53	0.97	0.97
	assign (segid 3A4 and resid 204 and name CA)	(segid 3A4 and resid 224 and name CA)	13.22	0.80	0.80
80	assign (segid 3A4 and resid 204 and name CA)	(segid 3A4 and resid 224 and name CB)	13.09	0.61	0.60
	assign (segid 3A4 and resid 204 and name CA)	(segid 3A4 and resid 225 and name CA)	10.54	1.05	1.05
	assign (segid 3A4 and resid 204 and name CA)	(segid 3A4 and resid 225 and name CB)	9.11	1.08	1.08
	assign (segid 3A4 and resid 204 and name CA)	(segid 3A4 and resid 226 and name CA)	12.70	1.45	1.46

	assign (segid 3A4 and resid 204 and name CA) (segid 3A4 and resid 240 and name CA)	15.46	0.70	0.70
	assign (segid 3A4 and resid 204 and name CA) (segid 3A4 and resid 240 and name CB)	16.58	0.76	0.76
	assign (segid 3A4 and resid 204 and name CA) (segid 3A4 and resid 241 and name CA)	12.48	0.81	0.81
	assign (segid 3A4 and resid 204 and name CA) (segid 3A4 and resid 241 and name CB)	11.94	0.93	0.94
	assign (segid 3A4 and resid 204 and name CA) (segid 3A4 and resid 242 and name CA)	15.05	0.88	0.88
5	assign (segid 3A4 and resid 204 and name CA) (segid 3A4 and resid 242 and name CB)	16.28	0.95	0.95
	assign (segid 3A4 and resid 204 and name CA) (segid 3A4 and resid 243 and name CA)	16.48	0.63	0.62
	assign (segid 3A4 and resid 204 and name CA) (segid 3A4 and resid 243 and name CB)	17.19	0.66	0.66
	assign (segid 3A4 and resid 204 and name CA) (segid 3A4 and resid 244 and name CA)	13.40	0.56	0.57
	assign (segid 3A4 and resid 204 and name CA) (segid 3A4 and resid 244 and name CB)	12.17	0.56	0.57
10	assign (segid 3A4 and resid 204 and name CA) (segid 3A4 and resid 245 and name CA)	13.03	0.58	0.58
	assign (segid 3A4 and resid 204 and name CA) (segid 3A4 and resid 245 and name CB)	12.98	0.60	0.61
	assign (segid 3A4 and resid 204 and name CA) (segid 3A4 and resid 246 and name CA)	16.73	0.62	0.62
	assign (segid 3A4 and resid 204 and name CA) (segid 3A4 and resid 246 and name CB)	17.80	0.60	0.59
	assign (segid 3A4 and resid 204 and name CA) (segid 3A4 and resid 247 and name CA)	16.86	0.47	0.47
	assign (segid 3A4 and resid 204 and name CA) (segid 3A4 and resid 247 and name CB)	16.57	0.42	0.43
15	assign (segid 3A4 and resid 204 and name CA) (segid 3A4 and resid 248 and name CA)	14.44	0.63	0.63
	assign (segid 3A4 and resid 204 and name CA) (segid 3A4 and resid 248 and name CB)	12.99	0.64	0.64
	assign (segid 3A4 and resid 204 and name CA) (segid 3A4 and resid 249 and name CA)	16.59	0.88	0.89
	assign (segid 3A4 and resid 204 and name CA) (segid 3A4 and resid 249 and name CB)	18.86	0.78	0.78
20	assign (segid 3A4 and resid 204 and name CA) (segid 3A4 and resid 251 and name CA)	17.82	0.73	0.72
	assign (segid 3A4 and resid 204 and name CA) (segid 3A4 and resid 251 and name CB)	18.36	1.09	1.08
	assign (segid 3A4 and resid 204 and name CA) (segid 3A4 and resid 252 and name CA)	17.34	1.13	1.12
	assign (segid 3A4 and resid 204 and name CA) (segid 3A4 and resid 252 and name CB)	5.52	0.05	0.06
	assign (segid 3A4 and resid 204 and name CB) (segid 3A4 and resid 205 and name C)	4.48	0.07	0.07
25	assign (segid 3A4 and resid 204 and name CB) (segid 3A4 and resid 205 and name CA)	5.26	0.13	0.13
	assign (segid 3A4 and resid 204 and name CB) (segid 3A4 and resid 205 and name CB)	3.20	0.09	0.08
	assign (segid 3A4 and resid 204 and name CB) (segid 3A4 and resid 205 and name N)	6.52	0.10	0.10
	assign (segid 3A4 and resid 204 and name CB) (segid 3A4 and resid 205 and name O)	7.00	0.06	0.07
	assign (segid 3A4 and resid 204 and name CB) (segid 3A4 and resid 206 and name C)	6.84	0.12	0.11
30	assign (segid 3A4 and resid 204 and name CB) (segid 3A4 and resid 206 and name CA)	7.28	0.18	0.17
	assign (segid 3A4 and resid 204 and name CB) (segid 3A4 and resid 206 and name CB)	5.60	0.09	0.09
	assign (segid 3A4 and resid 204 and name CB) (segid 3A4 and resid 206 and name N)	6.86	0.17	0.18
	assign (segid 3A4 and resid 204 and name CB) (segid 3A4 and resid 207 and name C)	6.61	0.12	0.11
	assign (segid 3A4 and resid 204 and name CB) (segid 3A4 and resid 207 and name CA)	6.01	0.24	0.23
35	assign (segid 3A4 and resid 204 and name CB) (segid 3A4 and resid 207 and name CB)	6.09	0.08	0.07
	assign (segid 3A4 and resid 204 and name CB) (segid 3A4 and resid 207 and name N)	12.74	0.72	0.73
	assign (segid 3A4 and resid 204 and name CB) (segid 3A4 and resid 209 and name CA)	11.63	0.67	0.67
	assign (segid 3A4 and resid 204 and name CB) (segid 3A4 and resid 219 and name CB)	13.67	0.71	0.71
	assign (segid 3A4 and resid 204 and name CB) (segid 3A4 and resid 220 and name CA)	14.40	0.62	0.63
40	assign (segid 3A4 and resid 204 and name CB) (segid 3A4 and resid 220 and name CB)	10.48	0.73	0.72
	assign (segid 3A4 and resid 204 and name CB) (segid 3A4 and resid 221 and name CA)	9.30	0.62	0.62
	assign (segid 3A4 and resid 204 and name CB) (segid 3A4 and resid 221 and name CB)	10.17	1.08	1.08
	assign (segid 3A4 and resid 204 and name CB) (segid 3A4 and resid 222 and name CA)	10.28	1.10	1.10
	assign (segid 3A4 and resid 204 and name CB) (segid 3A4 and resid 222 and name CB)	13.87	1.07	1.07
45	assign (segid 3A4 and resid 204 and name CB) (segid 3A4 and resid 223 and name CA)	14.94	1.04	1.03
	assign (segid 3A4 and resid 204 and name CB) (segid 3A4 and resid 223 and name CB)	13.84	0.91	0.91
	assign (segid 3A4 and resid 204 and name CB) (segid 3A4 and resid 224 and name CA)	13.61	0.71	0.71
	assign (segid 3A4 and resid 204 and name CB) (segid 3A4 and resid 224 and name CB)	11.44	1.16	1.17
	assign (segid 3A4 and resid 204 and name CB) (segid 3A4 and resid 225 and name CA)	10.01	1.19	1.20
50	assign (segid 3A4 and resid 204 and name CB) (segid 3A4 and resid 225 and name CB)	13.73	1.50	1.49
	assign (segid 3A4 and resid 204 and name CB) (segid 3A4 and resid 226 and name CA)	16.47	0.72	0.72
	assign (segid 3A4 and resid 204 and name CB) (segid 3A4 and resid 240 and name CA)	17.58	0.77	0.76
	assign (segid 3A4 and resid 204 and name CB) (segid 3A4 and resid 240 and name CB)	13.37	0.80	0.80
	assign (segid 3A4 and resid 204 and name CB) (segid 3A4 and resid 241 and name CA)	12.87	0.90	0.90
55	assign (segid 3A4 and resid 204 and name CB) (segid 3A4 and resid 241 and name CB)	15.69	0.83	0.83
	assign (segid 3A4 and resid 204 and name CB) (segid 3A4 and resid 242 and name CA)	16.95	0.89	0.88
	assign (segid 3A4 and resid 204 and name CB) (segid 3A4 and resid 242 and name CB)	17.09	0.65	0.65
	assign (segid 3A4 and resid 204 and name CB) (segid 3A4 and resid 243 and name CA)	17.89	0.70	0.69
	assign (segid 3A4 and resid 204 and name CB) (segid 3A4 and resid 243 and name CB)	13.94	0.62	0.63
60	assign (segid 3A4 and resid 204 and name CB) (segid 3A4 and resid 244 and name CA)	12.80	0.64	0.64
	assign (segid 3A4 and resid 204 and name CB) (segid 3A4 and resid 244 and name CB)	13.27	0.56	0.55
	assign (segid 3A4 and resid 204 and name CB) (segid 3A4 and resid 245 and name CA)	13.24	0.56	0.56
	assign (segid 3A4 and resid 204 and name CB) (segid 3A4 and resid 245 and name CB)	16.91	0.60	0.60
	assign (segid 3A4 and resid 204 and name CB) (segid 3A4 and resid 246 and name CA)	18.06	0.58	0.58
65	assign (segid 3A4 and resid 204 and name CB) (segid 3A4 and resid 246 and name CB)	17.02	0.52	0.51
	assign (segid 3A4 and resid 204 and name CB) (segid 3A4 and resid 247 and name CA)	16.83	0.51	0.50
	assign (segid 3A4 and resid 204 and name CB) (segid 3A4 and resid 247 and name CB)	14.33	0.61	0.61
	assign (segid 3A4 and resid 204 and name CB) (segid 3A4 and resid 248 and name CA)	12.88	0.60	0.59
	assign (segid 3A4 and resid 204 and name CB) (segid 3A4 and resid 248 and name CB)	16.32	0.85	0.85
70	assign (segid 3A4 and resid 204 and name CB) (segid 3A4 and resid 249 and name CA)	18.56	0.77	0.78
	assign (segid 3A4 and resid 204 and name CB) (segid 3A4 and resid 251 and name CA)	17.56	0.72	0.71
	assign (segid 3A4 and resid 204 and name CB) (segid 3A4 and resid 251 and name CB)	17.79	1.06	1.06
	assign (segid 3A4 and resid 204 and name CB) (segid 3A4 and resid 252 and name CA)	16.74	1.10	1.09
	assign (segid 3A4 and resid 204 and name CB) (segid 3A4 and resid 252 and name CB)	2.46	0.02	0.01
75	assign (segid 3A4 and resid 204 and name N) (segid 3A4 and resid 204 and name C)	1.46	0.01	0.00
	assign (segid 3A4 and resid 204 and name N) (segid 3A4 and resid 204 and name CA)	2.46	0.04	0.04
	assign (segid 3A4 and resid 204 and name N) (segid 3A4 and resid 204 and name CB)	3.52	0.02	0.03
	assign (segid 3A4 and resid 204 and name N) (segid 3A4 and resid 204 and name O)	4.76	0.02	0.03
	assign (segid 3A4 and resid 204 and name N) (segid 3A4 and resid 205 and name C)	4.17	0.05	0.06
80	assign (segid 3A4 and resid 204 and name N) (segid 3A4 and resid 205 and name CA)	4.92	0.08	0.08
	assign (segid 3A4 and resid 204 and name N) (segid 3A4 and resid 205 and name CB)	2.76	0.06	0.05
	assign (segid 3A4 and resid 204 and name N) (segid 3A4 and resid 205 and name N)	5.95	0.05	0.04
	assign (segid 3A4 and resid 204 and name N) (segid 3A4 and resid 205 and name O)			

	assign (segid 3A4 and resid 204 and name N)	(segid 3A4 and resid 206 and name C)	5.78	0.04	0.05
	assign (segid 3A4 and resid 204 and name N)	(segid 3A4 and resid 206 and name CA)	5.36	0.10	0.10
	assign (segid 3A4 and resid 204 and name N)	(segid 3A4 and resid 206 and name CB)	5.38	0.17	0.17
	assign (segid 3A4 and resid 204 and name N)	(segid 3A4 and resid 206 and name N)	4.30	0.08	0.09
	assign (segid 3A4 and resid 204 and name N)	(segid 3A4 and resid 206 and name O)	6.98	0.07	0.06
5	assign (segid 3A4 and resid 204 and name N)	(segid 3A4 and resid 207 and name C)	6.63	0.21	0.22
	assign (segid 3A4 and resid 204 and name N)	(segid 3A4 and resid 207 and name CA)	5.90	0.18	0.18
	assign (segid 3A4 and resid 204 and name N)	(segid 3A4 and resid 207 and name CB)	5.44	0.29	0.30
	assign (segid 3A4 and resid 204 and name N)	(segid 3A4 and resid 207 and name N)	5.06	0.10	0.09
	assign (segid 3A4 and resid 204 and name N)	(segid 3A4 and resid 204 and name CB)	3.21	0.04	0.05
10	assign (segid 3A4 and resid 204 and name O)	(segid 3A4 and resid 205 and name C)	3.19	0.10	0.10
	assign (segid 3A4 and resid 204 and name O)	(segid 3A4 and resid 205 and name CA)	2.77	0.03	0.04
	assign (segid 3A4 and resid 204 and name O)	(segid 3A4 and resid 205 and name CB)	4.21	0.04	0.03
	assign (segid 3A4 and resid 204 and name O)	(segid 3A4 and resid 205 and name N)	2.25	0.02	0.01
	assign (segid 3A4 and resid 204 and name O)	(segid 3A4 and resid 205 and name O)	3.89	0.20	0.21
15	assign (segid 3A4 and resid 204 and name O)	(segid 3A4 and resid 206 and name C)	4.32	0.08	0.08
	assign (segid 3A4 and resid 204 and name O)	(segid 3A4 and resid 206 and name CA)	4.52	0.10	0.10
	assign (segid 3A4 and resid 204 and name O)	(segid 3A4 and resid 206 and name CB)	5.44	0.13	0.14
	assign (segid 3A4 and resid 204 and name O)	(segid 3A4 and resid 206 and name N)	3.50	0.08	0.07
	assign (segid 3A4 and resid 204 and name O)	(segid 3A4 and resid 206 and name O)	5.32	0.08	0.08
20	assign (segid 3A4 and resid 204 and name O)	(segid 3A4 and resid 207 and name C)	3.87	0.22	0.21
	assign (segid 3A4 and resid 204 and name O)	(segid 3A4 and resid 207 and name CA)	3.90	0.12	0.11
	assign (segid 3A4 and resid 204 and name O)	(segid 3A4 and resid 207 and name CB)	3.85	0.14	0.14
	assign (segid 3A4 and resid 204 and name O)	(segid 3A4 and resid 207 and name N)	3.42	0.12	0.12
	assign (segid 3A4 and resid 204 and name O)	(segid 3A4 and resid 207 and name O)	4.97	0.13	0.14
25	assign (segid 3A4 and resid 205 and name C)	(segid 3A4 and resid 205 and name CB)	2.50	0.04	0.03
	assign (segid 3A4 and resid 205 and name C)	(segid 3A4 and resid 205 and name O)	1.23	0.00	0.01
	assign (segid 3A4 and resid 205 and name C)	(segid 3A4 and resid 206 and name C)	3.12	0.04	0.04
	assign (segid 3A4 and resid 205 and name C)	(segid 3A4 and resid 206 and name CA)	2.44	0.01	0.01
	assign (segid 3A4 and resid 205 and name C)	(segid 3A4 and resid 206 and name CB)	3.69	0.02	0.03
30	assign (segid 3A4 and resid 205 and name C)	(segid 3A4 and resid 206 and name N)	1.32	0.01	0.01
	assign (segid 3A4 and resid 205 and name C)	(segid 3A4 and resid 206 and name O)	4.04	0.09	0.10
	assign (segid 3A4 and resid 205 and name C)	(segid 3A4 and resid 207 and name C)	4.63	0.11	0.11
	assign (segid 3A4 and resid 205 and name C)	(segid 3A4 and resid 207 and name CA)	4.53	0.07	0.07
	assign (segid 3A4 and resid 205 and name C)	(segid 3A4 and resid 207 and name CB)	5.38	0.09	0.08
35	assign (segid 3A4 and resid 205 and name C)	(segid 3A4 and resid 207 and name N)	3.32	0.07	0.07
	assign (segid 3A4 and resid 205 and name C)	(segid 3A4 and resid 207 and name O)	5.64	0.17	0.17
	assign (segid 3A4 and resid 205 and name C)	(segid 3A4 and resid 225 and name CB)	5.47	0.80	0.79
	assign (segid 3A4 and resid 205 and name CA)	(segid 3A4 and resid 205 and name C)	1.52	0.01	0.01
	assign (segid 3A4 and resid 205 and name CA)	(segid 3A4 and resid 205 and name CB)	1.51	0.01	0.02
40	assign (segid 3A4 and resid 205 and name CA)	(segid 3A4 and resid 205 and name O)	2.40	0.01	0.00
	assign (segid 3A4 and resid 205 and name CA)	(segid 3A4 and resid 206 and name C)	4.45	0.04	0.04
	assign (segid 3A4 and resid 205 and name CA)	(segid 3A4 and resid 206 and name CA)	3.80	0.01	0.02
	assign (segid 3A4 and resid 205 and name CA)	(segid 3A4 and resid 206 and name CB)	4.84	0.02	0.03
	assign (segid 3A4 and resid 205 and name CA)	(segid 3A4 and resid 206 and name N)	2.42	0.01	0.01
45	assign (segid 3A4 and resid 205 and name CA)	(segid 3A4 and resid 206 and name O)	5.44	0.10	0.11
	assign (segid 3A4 and resid 205 and name CA)	(segid 3A4 and resid 207 and name C)	5.39	0.14	0.15
	assign (segid 3A4 and resid 205 and name CA)	(segid 3A4 and resid 207 and name CA)	5.40	0.07	0.07
	assign (segid 3A4 and resid 205 and name CA)	(segid 3A4 and resid 207 and name CB)	5.92	0.13	0.14
	assign (segid 3A4 and resid 205 and name CA)	(segid 3A4 and resid 207 and name N)	4.32	0.05	0.04
50	assign (segid 3A4 and resid 205 and name CA)	(segid 3A4 and resid 207 and name O)	6.45	0.17	0.17
	assign (segid 3A4 and resid 205 and name CA)	(segid 3A4 and resid 219 and name CA)	9.77	0.68	0.69
	assign (segid 3A4 and resid 205 and name CA)	(segid 3A4 and resid 219 and name CB)	9.04	0.61	0.60
	assign (segid 3A4 and resid 205 and name CA)	(segid 3A4 and resid 220 and name CA)	10.48	0.64	0.65
	assign (segid 3A4 and resid 205 and name CA)	(segid 3A4 and resid 220 and name CB)	11.49	0.62	0.62
55	assign (segid 3A4 and resid 205 and name CA)	(segid 3A4 and resid 221 and name CA)	7.38	0.52	0.52
	assign (segid 3A4 and resid 205 and name CA)	(segid 3A4 and resid 221 and name CB)	6.68	0.47	0.47
	assign (segid 3A4 and resid 205 and name CA)	(segid 3A4 and resid 222 and name CA)	6.07	0.98	0.98
	assign (segid 3A4 and resid 205 and name CA)	(segid 3A4 and resid 222 and name CB)	6.25	0.99	0.99
	assign (segid 3A4 and resid 205 and name CA)	(segid 3A4 and resid 223 and name CA)	9.68	1.02	1.03
60	assign (segid 3A4 and resid 205 and name CA)	(segid 3A4 and resid 223 and name CB)	10.87	0.99	1.00
	assign (segid 3A4 and resid 205 and name CA)	(segid 3A4 and resid 224 and name CA)	10.01	0.75	0.74
	assign (segid 3A4 and resid 205 and name CA)	(segid 3A4 and resid 224 and name CB)	10.09	0.54	0.54
	assign (segid 3A4 and resid 205 and name CA)	(segid 3A4 and resid 225 and name CA)	7.58	0.87	0.88
	assign (segid 3A4 and resid 205 and name CA)	(segid 3A4 and resid 225 and name CB)	6.12	0.88	0.88
65	assign (segid 3A4 and resid 205 and name CA)	(segid 3A4 and resid 226 and name CA)	9.45	1.37	1.37
	assign (segid 3A4 and resid 205 and name CA)	(segid 3A4 and resid 240 and name CA)	14.18	0.67	0.66
	assign (segid 3A4 and resid 205 and name CA)	(segid 3A4 and resid 240 and name CB)	15.49	0.71	0.70
	assign (segid 3A4 and resid 205 and name CA)	(segid 3A4 and resid 241 and name CA)	11.76	0.87	0.87
	assign (segid 3A4 and resid 205 and name CA)	(segid 3A4 and resid 241 and name CB)	11.63	0.99	0.99
70	assign (segid 3A4 and resid 205 and name CA)	(segid 3A4 and resid 242 and name CA)	14.55	0.88	0.89
	assign (segid 3A4 and resid 205 and name CA)	(segid 3A4 and resid 242 and name CB)	15.91	0.91	0.92
	assign (segid 3A4 and resid 205 and name CA)	(segid 3A4 and resid 243 and name CA)	15.13	0.63	0.63
	assign (segid 3A4 and resid 205 and name CA)	(segid 3A4 and resid 243 and name CB)	15.63	0.66	0.66
	assign (segid 3A4 and resid 205 and name CA)	(segid 3A4 and resid 244 and name CA)	11.71	0.60	0.60
75	assign (segid 3A4 and resid 205 and name CA)	(segid 3A4 and resid 244 and name CB)	10.45	0.62	0.61
	assign (segid 3A4 and resid 205 and name CA)	(segid 3A4 and resid 245 and name CA)	12.22	0.66	0.65
	assign (segid 3A4 and resid 205 and name CA)	(segid 3A4 and resid 245 and name CB)	12.59	0.68	0.68
	assign (segid 3A4 and resid 205 and name CA)	(segid 3A4 and resid 246 and name CA)	15.71	0.68	0.68
	assign (segid 3A4 and resid 205 and name CA)	(segid 3A4 and resid 246 and name CB)	16.77	0.64	0.64
80	assign (segid 3A4 and resid 205 and name CA)	(segid 3A4 and resid 247 and name CA)	15.06	0.54	0.53
	assign (segid 3A4 and resid 205 and name CA)	(segid 3A4 and resid 247 and name CB)	14.51	0.45	0.45
	assign (segid 3A4 and resid 205 and name CA)	(segid 3A4 and resid 248 and name CA)	12.85	0.76	0.76

	assign (segid 3A4 and resid 205 and name CA)	(segid 3A4 and resid 248 and name CB)	11.54	0.81	0.81
	assign (segid 3A4 and resid 205 and name CA)	(segid 3A4 and resid 249 and name CA)	15.67	0.95	0.95
	assign (segid 3A4 and resid 205 and name CA)	(segid 3A4 and resid 250 and name CA)	18.21	0.80	0.80
	assign (segid 3A4 and resid 205 and name CA)	(segid 3A4 and resid 250 and name CB)	18.56	0.66	0.65
	assign (segid 3A4 and resid 205 and name CA)	(segid 3A4 and resid 251 and name CA)	16.99	0.90	0.90
5	assign (segid 3A4 and resid 205 and name CA)	(segid 3A4 and resid 251 and name CB)	15.76	0.86	0.87
	assign (segid 3A4 and resid 205 and name CA)	(segid 3A4 and resid 252 and name CA)	17.09	1.20	1.20
	assign (segid 3A4 and resid 205 and name CA)	(segid 3A4 and resid 252 and name CB)	16.33	1.24	1.23
	assign (segid 3A4 and resid 205 and name CB)	(segid 3A4 and resid 206 and name C)	5.56	0.09	0.10
	assign (segid 3A4 and resid 205 and name CB)	(segid 3A4 and resid 206 and name CA)	4.62	0.11	0.11
10	assign (segid 3A4 and resid 205 and name CB)	(segid 3A4 and resid 206 and name CB)	5.51	0.13	0.13
	assign (segid 3A4 and resid 205 and name CB)	(segid 3A4 and resid 206 and name N)	3.30	0.11	0.12
	assign (segid 3A4 and resid 205 and name CB)	(segid 3A4 and resid 206 and name O)	6.50	0.13	0.13
	assign (segid 3A4 and resid 205 and name CB)	(segid 3A4 and resid 207 and name C)	6.82	0.13	0.14
	assign (segid 3A4 and resid 205 and name CB)	(segid 3A4 and resid 207 and name CA)	6.82	0.09	0.08
15	assign (segid 3A4 and resid 205 and name CB)	(segid 3A4 and resid 207 and name CB)	7.39	0.16	0.16
	assign (segid 3A4 and resid 205 and name CB)	(segid 3A4 and resid 207 and name N)	5.64	0.08	0.09
	assign (segid 3A4 and resid 205 and name CB)	(segid 3A4 and resid 207 and name O)	8.68	0.68	0.67
	assign (segid 3A4 and resid 205 and name CB)	(segid 3A4 and resid 219 and name CB)	7.95	0.59	0.58
	assign (segid 3A4 and resid 205 and name CB)	(segid 3A4 and resid 219 and name CG)	6.49	0.59	0.59
20	assign (segid 3A4 and resid 205 and name CB)	(segid 3A4 and resid 219 and name CA)	9.11	0.67	0.66
	assign (segid 3A4 and resid 205 and name CB)	(segid 3A4 and resid 220 and name CA)	10.06	0.64	0.63
	assign (segid 3A4 and resid 205 and name CB)	(segid 3A4 and resid 220 and name CB)	5.29	0.71	0.71
	assign (segid 3A4 and resid 205 and name CB)	(segid 3A4 and resid 221 and name C)	5.93	0.54	0.53
	assign (segid 3A4 and resid 205 and name CB)	(segid 3A4 and resid 221 and name CB)	5.21	0.48	0.48
25	assign (segid 3A4 and resid 205 and name CB)	(segid 3A4 and resid 221 and name O)	5.46	0.71	0.72
	assign (segid 3A4 and resid 205 and name CB)	(segid 3A4 and resid 222 and name CA)	5.04	1.03	1.02
	assign (segid 3A4 and resid 205 and name CB)	(segid 3A4 and resid 222 and name CB)	5.42	1.01	1.01
	assign (segid 3A4 and resid 205 and name CB)	(segid 3A4 and resid 222 and name N)	5.10	0.87	0.86
	assign (segid 3A4 and resid 205 and name CB)	(segid 3A4 and resid 223 and name CA)	8.66	1.01	1.01
30	assign (segid 3A4 and resid 205 and name CB)	(segid 3A4 and resid 223 and name CB)	9.77	0.99	0.99
	assign (segid 3A4 and resid 205 and name CB)	(segid 3A4 and resid 224 and name CA)	8.86	0.73	0.73
	assign (segid 3A4 and resid 205 and name CB)	(segid 3A4 and resid 224 and name CB)	8.83	0.53	0.52
	assign (segid 3A4 and resid 205 and name CB)	(segid 3A4 and resid 225 and name CA)	6.83	0.86	0.85
	assign (segid 3A4 and resid 205 and name CB)	(segid 3A4 and resid 225 and name CB)	5.43	0.89	0.89
35	assign (segid 3A4 and resid 205 and name CB)	(segid 3A4 and resid 225 and name CA)	9.04	1.29	1.28
	assign (segid 3A4 and resid 205 and name CB)	(segid 3A4 and resid 226 and name CA)	13.59	0.50	0.50
	assign (segid 3A4 and resid 205 and name CB)	(segid 3A4 and resid 240 and name CA)	14.91	0.53	0.53
	assign (segid 3A4 and resid 205 and name CB)	(segid 3A4 and resid 240 and name CB)	11.20	0.75	0.75
	assign (segid 3A4 and resid 205 and name CB)	(segid 3A4 and resid 241 and name CA)	11.23	0.89	0.90
40	assign (segid 3A4 and resid 205 and name CB)	(segid 3A4 and resid 241 and name CB)	13.81	0.78	0.78
	assign (segid 3A4 and resid 205 and name CB)	(segid 3A4 and resid 242 and name CA)	15.22	0.80	0.80
	assign (segid 3A4 and resid 205 and name CB)	(segid 3A4 and resid 242 and name CB)	14.15	0.49	0.48
	assign (segid 3A4 and resid 205 and name CB)	(segid 3A4 and resid 243 and name CA)	14.66	0.49	0.49
	assign (segid 3A4 and resid 205 and name CB)	(segid 3A4 and resid 243 and name CB)	10.61	0.47	0.48
45	assign (segid 3A4 and resid 205 and name CB)	(segid 3A4 and resid 244 and name CA)	9.42	0.48	0.48
	assign (segid 3A4 and resid 205 and name CB)	(segid 3A4 and resid 244 and name CB)	11.15	0.60	0.60
	assign (segid 3A4 and resid 205 and name CB)	(segid 3A4 and resid 245 and name CA)	11.66	0.61	0.61
	assign (segid 3A4 and resid 205 and name CB)	(segid 3A4 and resid 245 and name CB)	14.54	0.63	0.62
	assign (segid 3A4 and resid 205 and name CB)	(segid 3A4 and resid 246 and name CA)	15.63	0.57	0.56
50	assign (segid 3A4 and resid 205 and name CB)	(segid 3A4 and resid 246 and name CB)	13.70	0.48	0.49
	assign (segid 3A4 and resid 205 and name CB)	(segid 3A4 and resid 247 and name CA)	13.16	0.39	0.39
	assign (segid 3A4 and resid 205 and name CB)	(segid 3A4 and resid 247 and name CB)	11.45	0.76	0.76
	assign (segid 3A4 and resid 205 and name CB)	(segid 3A4 and resid 248 and name CA)	10.18	0.81	0.82
	assign (segid 3A4 and resid 205 and name CB)	(segid 3A4 and resid 248 and name CB)	14.38	0.95	0.95
55	assign (segid 3A4 and resid 205 and name CB)	(segid 3A4 and resid 249 and name CA)	16.81	0.79	0.79
	assign (segid 3A4 and resid 205 and name CB)	(segid 3A4 and resid 250 and name CA)	17.16	0.63	0.63
	assign (segid 3A4 and resid 205 and name CB)	(segid 3A4 and resid 251 and name CA)	15.52	0.91	0.91
	assign (segid 3A4 and resid 205 and name CB)	(segid 3A4 and resid 251 and name CB)	14.29	0.88	0.87
	assign (segid 3A4 and resid 205 and name CB)	(segid 3A4 and resid 252 and name CA)	15.71	1.22	1.23
60	assign (segid 3A4 and resid 205 and name CB)	(segid 3A4 and resid 252 and name CB)	15.00	1.26	1.26
	assign (segid 3A4 and resid 205 and name CB)	(segid 3A4 and resid 205 and name C)	2.47	0.02	0.02
	assign (segid 3A4 and resid 205 and name N)	(segid 3A4 and resid 205 and name CA)	1.45	0.01	0.01
	assign (segid 3A4 and resid 205 and name N)	(segid 3A4 and resid 205 and name CB)	2.43	0.03	0.04
	assign (segid 3A4 and resid 205 and name N)	(segid 3A4 and resid 205 and name O)	3.57	0.03	0.04
65	assign (segid 3A4 and resid 205 and name N)	(segid 3A4 and resid 206 and name C)	4.72	0.02	0.02
	assign (segid 3A4 and resid 205 and name N)	(segid 3A4 and resid 206 and name CA)	4.16	0.07	0.06
	assign (segid 3A4 and resid 205 and name N)	(segid 3A4 and resid 206 and name CB)	4.87	0.09	0.10
	assign (segid 3A4 and resid 205 and name N)	(segid 3A4 and resid 206 and name N)	2.73	0.06	0.06
	assign (segid 3A4 and resid 205 and name N)	(segid 3A4 and resid 206 and name O)	5.86	0.05	0.05
70	assign (segid 3A4 and resid 205 and name N)	(segid 3A4 and resid 207 and name C)	5.57	0.17	0.16
	assign (segid 3A4 and resid 205 and name N)	(segid 3A4 and resid 207 and name CA)	5.32	0.10	0.10
	assign (segid 3A4 and resid 205 and name N)	(segid 3A4 and resid 207 and name CB)	5.49	0.20	0.19
	assign (segid 3A4 and resid 205 and name N)	(segid 3A4 and resid 207 and name N)	6.28	0.04	0.05
	assign (segid 3A4 and resid 205 and name N)	(segid 3A4 and resid 207 and name O)	6.71	0.13	0.13
75	assign (segid 3A4 and resid 205 and name O)	(segid 3A4 and resid 205 and name CB)	3.14	0.09	0.09
	assign (segid 3A4 and resid 205 and name O)	(segid 3A4 and resid 206 and name C)	3.21	0.09	0.08
	assign (segid 3A4 and resid 205 and name O)	(segid 3A4 and resid 206 and name CA)	2.77	0.01	0.01
	assign (segid 3A4 and resid 205 and name O)	(segid 3A4 and resid 206 and name CB)	4.22	0.02	0.03
80	assign (segid 3A4 and resid 205 and name O)	(segid 3A4 and resid 206 and name N)	2.25	0.01	0.01
	assign (segid 3A4 and resid 205 and name O)	(segid 3A4 and resid 206 and name O)	3.80	0.10	0.11
	assign (segid 3A4 and resid 205 and name O)	(segid 3A4 and resid 207 and name C)	4.48	0.23	0.23
	assign (segid 3A4 and resid 205 and name O)	(segid 3A4 and resid 207 and name CA)	4.67	0.21	0.20

	assign (segid 3A4 and resid 205 and name O) (segid 3A4 and resid 207 and name CB)	5.75	0.17	0.18
	assign (segid 3A4 and resid 205 and name O) (segid 3A4 and resid 207 and name N)	3.63	0.19	0.19
	assign (segid 3A4 and resid 205 and name O) (segid 3A4 and resid 207 and name O)	5.32	0.26	0.26
	assign (segid 3A4 and resid 205 and name O) (segid 3A4 and resid 225 and name CB)	5.39	0.73	0.74
5	assign (segid 3A4 and resid 206 and name C) (segid 3A4 and resid 206 and name CB)	2.48	0.02	0.02
	assign (segid 3A4 and resid 206 and name C) (segid 3A4 and resid 206 and name O)	1.23	0.00	0.00
	assign (segid 3A4 and resid 206 and name C) (segid 3A4 and resid 207 and name C)	3.19	0.09	0.08
	assign (segid 3A4 and resid 206 and name C) (segid 3A4 and resid 207 and name CA)	2.44	0.01	0.01
	assign (segid 3A4 and resid 206 and name C) (segid 3A4 and resid 207 and name CB)	3.69	0.06	0.05
	assign (segid 3A4 and resid 206 and name C) (segid 3A4 and resid 207 and name N)	1.33	0.01	0.00
10	assign (segid 3A4 and resid 206 and name C) (segid 3A4 and resid 207 and name O)	4.02	0.18	0.18
	assign (segid 3A4 and resid 206 and name C) (segid 3A4 and resid 225 and name CB)	6.75	0.57	0.57
	assign (segid 3A4 and resid 206 and name C) (segid 3A4 and resid 206 and name C)	1.53	0.01	0.01
	assign (segid 3A4 and resid 206 and name CA) (segid 3A4 and resid 206 and name CB)	1.52	0.01	0.01
	assign (segid 3A4 and resid 206 and name CA) (segid 3A4 and resid 206 and name O)	2.41	0.01	0.01
15	assign (segid 3A4 and resid 206 and name CA) (segid 3A4 and resid 207 and name C)	4.51	0.04	0.05
	assign (segid 3A4 and resid 206 and name CA) (segid 3A4 and resid 207 and name CA)	3.81	0.02	0.02
	assign (segid 3A4 and resid 206 and name CA) (segid 3A4 and resid 207 and name CB)	4.85	0.03	0.02
	assign (segid 3A4 and resid 206 and name CA) (segid 3A4 and resid 207 and name N)	2.43	0.02	0.03
	assign (segid 3A4 and resid 206 and name CA) (segid 3A4 and resid 207 and name O)	5.42	0.16	0.16
20	assign (segid 3A4 and resid 206 and name CA) (segid 3A4 and resid 219 and name CA)	12.36	0.57	0.56
	assign (segid 3A4 and resid 206 and name CA) (segid 3A4 and resid 219 and name CB)	11.96	0.50	0.50
	assign (segid 3A4 and resid 206 and name CA) (segid 3A4 and resid 220 and name CA)	12.50	0.49	0.50
	assign (segid 3A4 and resid 206 and name CA) (segid 3A4 and resid 220 and name CB)	13.58	0.48	0.48
	assign (segid 3A4 and resid 206 and name CA) (segid 3A4 and resid 221 and name CA)	9.31	0.41	0.41
25	assign (segid 3A4 and resid 206 and name CA) (segid 3A4 and resid 221 and name CB)	9.02	0.49	0.49
	assign (segid 3A4 and resid 206 and name CA) (segid 3A4 and resid 222 and name CA)	7.47	0.68	0.67
	assign (segid 3A4 and resid 206 and name CA) (segid 3A4 and resid 222 and name CB)	7.93	0.67	0.66
	assign (segid 3A4 and resid 206 and name CA) (segid 3A4 and resid 223 and name CA)	10.26	0.89	0.88
	assign (segid 3A4 and resid 206 and name CA) (segid 3A4 and resid 223 and name CB)	11.70	0.86	0.85
30	assign (segid 3A4 and resid 206 and name CA) (segid 3A4 and resid 224 and name CA)	10.06	0.63	0.64
	assign (segid 3A4 and resid 206 and name CA) (segid 3A4 and resid 224 and name CB)	10.42	0.47	0.48
	assign (segid 3A4 and resid 206 and name CA) (segid 3A4 and resid 225 and name CA)	6.68	0.71	0.71
	assign (segid 3A4 and resid 206 and name CA) (segid 3A4 and resid 225 and name CB)	5.44	0.62	0.62
35	assign (segid 3A4 and resid 206 and name CA) (segid 3A4 and resid 226 and name CA)	7.91	1.40	1.40
	assign (segid 3A4 and resid 206 and name CA) (segid 3A4 and resid 240 and name CA)	12.36	0.97	0.97
	assign (segid 3A4 and resid 206 and name CA) (segid 3A4 and resid 240 and name CB)	13.68	1.01	1.02
	assign (segid 3A4 and resid 206 and name CA) (segid 3A4 and resid 241 and name CA)	10.44	1.14	1.14
	assign (segid 3A4 and resid 206 and name CA) (segid 3A4 and resid 241 and name CB)	10.16	1.25	1.25
40	assign (segid 3A4 and resid 206 and name CA) (segid 3A4 and resid 242 and name CA)	13.81	1.13	1.14
	assign (segid 3A4 and resid 206 and name CA) (segid 3A4 and resid 242 and name CB)	15.01	1.17	1.18
	assign (segid 3A4 and resid 206 and name CA) (segid 3A4 and resid 243 and name CA)	14.58	0.95	0.95
	assign (segid 3A4 and resid 206 and name CA) (segid 3A4 and resid 243 and name CB)	14.84	1.00	0.99
	assign (segid 3A4 and resid 206 and name CA) (segid 3A4 and resid 244 and name CA)	11.65	0.88	0.87
	assign (segid 3A4 and resid 206 and name CA) (segid 3A4 and resid 244 and name CB)	10.20	0.88	0.88
45	assign (segid 3A4 and resid 206 and name CA) (segid 3A4 and resid 245 and name CA)	12.82	0.92	0.91
	assign (segid 3A4 and resid 206 and name CA) (segid 3A4 and resid 245 and name CB)	13.03	0.96	0.95
	assign (segid 3A4 and resid 206 and name CA) (segid 3A4 and resid 246 and name CA)	16.31	0.92	0.93
	assign (segid 3A4 and resid 206 and name CA) (segid 3A4 and resid 246 and name CB)	17.10	0.91	0.91
	assign (segid 3A4 and resid 206 and name CA) (segid 3A4 and resid 247 and name CA)	15.93	0.77	0.76
50	assign (segid 3A4 and resid 206 and name CA) (segid 3A4 and resid 247 and name CB)	15.21	0.68	0.68
	assign (segid 3A4 and resid 206 and name CA) (segid 3A4 and resid 248 and name CA)	14.51	0.93	0.92
	assign (segid 3A4 and resid 206 and name CA) (segid 3A4 and resid 248 and name CB)	13.26	1.00	1.00
	assign (segid 3A4 and resid 206 and name CA) (segid 3A4 and resid 249 and name CA)	17.40	1.06	1.05
	assign (segid 3A4 and resid 206 and name CA) (segid 3A4 and resid 251 and name CB)	17.78	0.96	0.96
55	assign (segid 3A4 and resid 206 and name CB) (segid 3A4 and resid 207 and name C)	5.55	0.08	0.08
	assign (segid 3A4 and resid 206 and name CB) (segid 3A4 and resid 207 and name CA)	4.51	0.06	0.07
	assign (segid 3A4 and resid 206 and name CB) (segid 3A4 and resid 207 and name CB)	5.30	0.04	0.04
	assign (segid 3A4 and resid 206 and name CB) (segid 3A4 and resid 207 and name N)	3.20	0.08	0.08
	assign (segid 3A4 and resid 206 and name CB) (segid 3A4 and resid 207 and name O)	6.44	0.17	0.17
60	assign (segid 3A4 and resid 206 and name CB) (segid 3A4 and resid 219 and name CA)	13.43	0.48	0.48
	assign (segid 3A4 and resid 206 and name CB) (segid 3A4 and resid 219 and name CB)	13.01	0.42	0.43
	assign (segid 3A4 and resid 206 and name CB) (segid 3A4 and resid 220 and name CA)	13.23	0.41	0.41
	assign (segid 3A4 and resid 206 and name CB) (segid 3A4 and resid 220 and name CB)	14.21	0.40	0.41
	assign (segid 3A4 and resid 206 and name CB) (segid 3A4 and resid 221 and name CA)	9.87	0.35	0.35
65	assign (segid 3A4 and resid 206 and name CB) (segid 3A4 and resid 221 and name CB)	9.56	0.44	0.45
	assign (segid 3A4 and resid 206 and name CB) (segid 3A4 and resid 222 and name CA)	8.42	0.60	0.59
	assign (segid 3A4 and resid 206 and name CB) (segid 3A4 and resid 222 and name CB)	9.06	0.58	0.58
	assign (segid 3A4 and resid 206 and name CB) (segid 3A4 and resid 223 and name CA)	10.99	0.80	0.79
	assign (segid 3A4 and resid 206 and name CB) (segid 3A4 and resid 223 and name CB)	12.44	0.76	0.75
70	assign (segid 3A4 and resid 206 and name CB) (segid 3A4 and resid 224 and name CA)	10.29	0.59	0.59
	assign (segid 3A4 and resid 206 and name CB) (segid 3A4 and resid 224 and name CB)	10.56	0.42	0.42
	assign (segid 3A4 and resid 206 and name CB) (segid 3A4 and resid 225 and name CA)	6.76	0.72	0.71
	assign (segid 3A4 and resid 206 and name CB) (segid 3A4 and resid 225 and name CB)	5.67	0.61	0.61
	assign (segid 3A4 and resid 206 and name CB) (segid 3A4 and resid 226 and name CA)	8.26	1.39	1.39
75	assign (segid 3A4 and resid 206 and name CB) (segid 3A4 and resid 240 and name CA)	11.32	1.02	1.02
	assign (segid 3A4 and resid 206 and name CB) (segid 3A4 and resid 240 and name CB)	12.59	1.08	1.08
	assign (segid 3A4 and resid 206 and name CB) (segid 3A4 and resid 241 and name CA)	9.34	1.19	1.18
	assign (segid 3A4 and resid 206 and name CB) (segid 3A4 and resid 241 and name CB)	8.94	1.30	1.30
80	assign (segid 3A4 and resid 206 and name CB) (segid 3A4 and resid 242 and name CA)	12.77	1.19	1.19
	assign (segid 3A4 and resid 206 and name CB) (segid 3A4 and resid 242 and name CB)	13.90	1.24	1.24
	assign (segid 3A4 and resid 206 and name CB) (segid 3A4 and resid 243 and name CA)	13.80	1.01	1.00
	assign (segid 3A4 and resid 206 and name CB) (segid 3A4 and resid 243 and name CB)	14.06	1.04	1.05

	assign (segid 3A4 and resid 206 and name CB)	(segid 3A4 and resid 244 and name CA)	11.11	0.91	0.91
	assign (segid 3A4 and resid 206 and name CB)	(segid 3A4 and resid 244 and name CB)	9.64	0.90	0.90
	assign (segid 3A4 and resid 206 and name CB)	(segid 3A4 and resid 245 and name CA)	12.22	0.97	0.97
	assign (segid 3A4 and resid 206 and name CB)	(segid 3A4 and resid 245 and name CB)	12.30	1.02	1.03
5	assign (segid 3A4 and resid 206 and name CB)	(segid 3A4 and resid 246 and name CA)	15.74	0.98	0.98
	assign (segid 3A4 and resid 206 and name CB)	(segid 3A4 and resid 246 and name CB)	16.44	0.96	0.97
	assign (segid 3A4 and resid 206 and name CB)	(segid 3A4 and resid 247 and name CA)	15.65	0.81	0.80
	assign (segid 3A4 and resid 206 and name CB)	(segid 3A4 and resid 247 and name CB)	14.97	0.71	0.71
	assign (segid 3A4 and resid 206 and name CB)	(segid 3A4 and resid 248 and name CA)	14.44	0.94	0.93
10	assign (segid 3A4 and resid 206 and name CB)	(segid 3A4 and resid 248 and name CB)	13.18	1.01	1.01
	assign (segid 3A4 and resid 206 and name CB)	(segid 3A4 and resid 249 and name CA)	17.17	1.08	1.08
	assign (segid 3A4 and resid 206 and name CB)	(segid 3A4 and resid 251 and name CB)	17.97	0.96	0.95
	assign (segid 3A4 and resid 206 and name N)	(segid 3A4 and resid 206 and name C)	2.46	0.05	0.04
	assign (segid 3A4 and resid 206 and name N)	(segid 3A4 and resid 206 and name CA)	1.46	0.00	0.01
15	assign (segid 3A4 and resid 206 and name N)	(segid 3A4 and resid 206 and name CB)	2.46	0.03	0.02
	assign (segid 3A4 and resid 206 and name N)	(segid 3A4 and resid 206 and name O)	3.54	0.07	0.06
	assign (segid 3A4 and resid 206 and name N)	(segid 3A4 and resid 207 and name C)	4.67	0.09	0.09
	assign (segid 3A4 and resid 206 and name N)	(segid 3A4 and resid 207 and name CA)	4.15	0.09	0.08
20	assign (segid 3A4 and resid 206 and name N)	(segid 3A4 and resid 207 and name CB)	4.93	0.12	0.13
	assign (segid 3A4 and resid 206 and name N)	(segid 3A4 and resid 207 and name N)	2.74	0.07	0.08
	assign (segid 3A4 and resid 206 and name N)	(segid 3A4 and resid 207 and name O)	5.73	0.16	0.16
	assign (segid 3A4 and resid 206 and name N)	(segid 3A4 and resid 225 and name CB)	5.44	0.80	0.80
	assign (segid 3A4 and resid 206 and name O)	(segid 3A4 and resid 206 and name CB)	3.19	0.08	0.09
	assign (segid 3A4 and resid 206 and name O)	(segid 3A4 and resid 207 and name C)	3.31	0.18	0.18
25	assign (segid 3A4 and resid 206 and name O)	(segid 3A4 and resid 207 and name CA)	2.78	0.05	0.04
	assign (segid 3A4 and resid 206 and name O)	(segid 3A4 and resid 207 and name CB)	4.19	0.15	0.14
	assign (segid 3A4 and resid 206 and name O)	(segid 3A4 and resid 207 and name N)	2.24	0.02	0.03
	assign (segid 3A4 and resid 206 and name O)	(segid 3A4 and resid 207 and name O)	3.81	0.30	0.29
30	assign (segid 3A4 and resid 207 and name C)	(segid 3A4 and resid 207 and name CB)	2.49	0.01	0.02
	assign (segid 3A4 and resid 207 and name C)	(segid 3A4 and resid 207 and name O)	1.23	0.01	0.01
	assign (segid 3A4 and resid 207 and name CA)	(segid 3A4 and resid 207 and name C)	1.53	0.01	0.00
	assign (segid 3A4 and resid 207 and name CA)	(segid 3A4 and resid 207 and name CB)	1.54	0.01	0.01
	assign (segid 3A4 and resid 207 and name CA)	(segid 3A4 and resid 207 and name O)	2.39	0.03	0.03
35	assign (segid 3A4 and resid 207 and name CA)	(segid 3A4 and resid 219 and name CA)	14.39	0.83	0.83
	assign (segid 3A4 and resid 207 and name CA)	(segid 3A4 and resid 219 and name CB)	13.84	0.74	0.75
	assign (segid 3A4 and resid 207 and name CA)	(segid 3A4 and resid 220 and name CA)	15.32	0.65	0.66
	assign (segid 3A4 and resid 207 and name CA)	(segid 3A4 and resid 220 and name CB)	16.47	0.60	0.61
	assign (segid 3A4 and resid 207 and name CA)	(segid 3A4 and resid 221 and name CA)	12.35	0.48	0.47
40	assign (segid 3A4 and resid 207 and name CA)	(segid 3A4 and resid 221 and name CB)	11.86	0.46	0.46
	assign (segid 3A4 and resid 207 and name CA)	(segid 3A4 and resid 222 and name CA)	10.19	0.87	0.86
	assign (segid 3A4 and resid 207 and name CA)	(segid 3A4 and resid 222 and name CB)	10.16	0.92	0.92
	assign (segid 3A4 and resid 207 and name CA)	(segid 3A4 and resid 223 and name CA)	13.24	1.02	1.03
	assign (segid 3A4 and resid 207 and name CA)	(segid 3A4 and resid 223 and name CB)	14.64	1.02	1.02
45	assign (segid 3A4 and resid 207 and name CA)	(segid 3A4 and resid 224 and name CA)	13.63	0.65	0.66
	assign (segid 3A4 and resid 207 and name CA)	(segid 3A4 and resid 224 and name CB)	14.04	0.48	0.49
	assign (segid 3A4 and resid 207 and name CA)	(segid 3A4 and resid 225 and name CA)	10.34	0.68	0.68
	assign (segid 3A4 and resid 207 and name CA)	(segid 3A4 and resid 225 and name CB)	9.04	0.61	0.61
	assign (segid 3A4 and resid 207 and name CA)	(segid 3A4 and resid 226 and name CA)	10.98	1.35	1.36
	assign (segid 3A4 and resid 207 and name CA)	(segid 3A4 and resid 240 and name CA)	15.75	1.10	1.11
50	assign (segid 3A4 and resid 207 and name CA)	(segid 3A4 and resid 240 and name CB)	16.99	1.19	1.19
	assign (segid 3A4 and resid 207 and name CA)	(segid 3A4 and resid 241 and name CA)	13.70	1.23	1.24
	assign (segid 3A4 and resid 207 and name CA)	(segid 3A4 and resid 241 and name CB)	13.17	1.38	1.38
	assign (segid 3A4 and resid 207 and name CA)	(segid 3A4 and resid 243 and name CA)	18.16	0.99	1.00
	assign (segid 3A4 and resid 207 and name CA)	(segid 3A4 and resid 243 and name CB)	18.48	1.04	1.03
55	assign (segid 3A4 and resid 207 and name CA)	(segid 3A4 and resid 244 and name CA)	15.29	0.87	0.86
	assign (segid 3A4 and resid 207 and name CA)	(segid 3A4 and resid 244 and name CB)	13.85	0.86	0.87
	assign (segid 3A4 and resid 207 and name CA)	(segid 3A4 and resid 245 and name CA)	16.07	0.94	0.93
	assign (segid 3A4 and resid 207 and name CA)	(segid 3A4 and resid 245 and name CB)	16.12	0.99	1.00
	assign (segid 3A4 and resid 207 and name CA)	(segid 3A4 and resid 248 and name CA)	17.72	0.87	0.87
60	assign (segid 3A4 and resid 207 and name CA)	(segid 3A4 and resid 248 and name CB)	16.39	0.93	0.93
	assign (segid 3A4 and resid 207 and name CB)	(segid 3A4 and resid 219 and name CA)	15.22	0.79	0.80
	assign (segid 3A4 and resid 207 and name CB)	(segid 3A4 and resid 219 and name CB)	14.55	0.73	0.73
	assign (segid 3A4 and resid 207 and name CB)	(segid 3A4 and resid 220 and name CA)	16.21	0.60	0.61
	assign (segid 3A4 and resid 207 and name CB)	(segid 3A4 and resid 220 and name CB)	17.30	0.56	0.56
65	assign (segid 3A4 and resid 207 and name CB)	(segid 3A4 and resid 221 and name CA)	13.13	0.44	0.44
	assign (segid 3A4 and resid 207 and name CB)	(segid 3A4 and resid 221 and name CB)	12.49	0.41	0.42
	assign (segid 3A4 and resid 207 and name CB)	(segid 3A4 and resid 222 and name CA)	11.25	0.86	0.86
	assign (segid 3A4 and resid 207 and name CB)	(segid 3A4 and resid 222 and name CB)	11.23	0.93	0.93
	assign (segid 3A4 and resid 207 and name CB)	(segid 3A4 and resid 223 and name CA)	14.47	0.99	0.98
70	assign (segid 3A4 and resid 207 and name CB)	(segid 3A4 and resid 223 and name CB)	15.84	0.98	0.97
	assign (segid 3A4 and resid 207 and name CB)	(segid 3A4 and resid 224 and name CA)	14.73	0.63	0.64
	assign (segid 3A4 and resid 207 and name CB)	(segid 3A4 and resid 224 and name CB)	15.03	0.44	0.45
	assign (segid 3A4 and resid 207 and name CB)	(segid 3A4 and resid 225 and name CA)	11.45	0.71	0.71
	assign (segid 3A4 and resid 207 and name CB)	(segid 3A4 and resid 225 and name CB)	10.12	0.65	0.65
75	assign (segid 3A4 and resid 207 and name CB)	(segid 3A4 and resid 226 and name CA)	12.37	1.37	1.36
	assign (segid 3A4 and resid 207 and name CB)	(segid 3A4 and resid 240 and name CA)	16.43	1.09	1.09
	assign (segid 3A4 and resid 207 and name CB)	(segid 3A4 and resid 240 and name CB)	17.61	1.20	1.19
	assign (segid 3A4 and resid 207 and name CB)	(segid 3A4 and resid 241 and name CA)	14.14	1.23	1.23
80	assign (segid 3A4 and resid 207 and name CB)	(segid 3A4 and resid 241 and name CB)	13.49	1.37	1.37
	assign (segid 3A4 and resid 207 and name CB)	(segid 3A4 and resid 241 and name CA)	15.91	0.87	0.87
	assign (segid 3A4 and resid 207 and name CB)	(segid 3A4 and resid 244 and name CB)	14.49	0.85	0.86
	assign (segid 3A4 and resid 207 and name CB)	(segid 3A4 and resid 245 and name CA)	16.36	0.99	0.98
	assign (segid 3A4 and resid 207 and name CB)	(segid 3A4 and resid 245 and name CB)	16.30	1.05	1.06

	assign (segid 3A4 and resid 207 and name CB)	(segid 3A4 and resid 248 and name CA)	18.15	0.88	0.89
	assign (segid 3A4 and resid 207 and name CB)	(segid 3A4 and resid 248 and name CB)	16.77	0.94	0.95
	assign (segid 3A4 and resid 207 and name N)	(segid 3A4 and resid 207 and name C)	2.45	0.03	0.03
	assign (segid 3A4 and resid 207 and name N)	(segid 3A4 and resid 207 and name CA)	1.46	0.01	0.00
	assign (segid 3A4 and resid 207 and name N)	(segid 3A4 and resid 207 and name CB)	2.47	0.02	0.02
5	assign (segid 3A4 and resid 207 and name N)	(segid 3A4 and resid 207 and name O)	3.48	0.06	0.06
	assign (segid 3A4 and resid 207 and name N)	(segid 3A4 and resid 207 and name CB)	3.24	0.16	0.16
	assign (segid 3A4 and resid 207 and name O)	(segid 3A4 and resid 20 and name CB)	2.52	0.04	0.03
	assign (segid 3A4 and resid 20 and name C)	(segid 3A4 and resid 20 and name O)	1.24	0.01	0.00
	assign (segid 3A4 and resid 20 and name C)	(segid 3A4 and resid 20 and name C)	3.55	0.04	0.03
10	assign (segid 3A4 and resid 20 and name C)	(segid 3A4 and resid 21 and name CA)	2.40	0.03	0.03
	assign (segid 3A4 and resid 20 and name C)	(segid 3A4 and resid 21 and name CB)	3.29	0.11	0.11
	assign (segid 3A4 and resid 20 and name C)	(segid 3A4 and resid 21 and name N)	1.32	0.01	0.01
	assign (segid 3A4 and resid 20 and name C)	(segid 3A4 and resid 21 and name O)	3.83	0.11	0.10
	assign (segid 3A4 and resid 20 and name C)	(segid 3A4 and resid 22 and name C)	6.79	0.12	0.13
15	assign (segid 3A4 and resid 20 and name C)	(segid 3A4 and resid 22 and name CA)	5.87	0.07	0.06
	assign (segid 3A4 and resid 20 and name C)	(segid 3A4 and resid 22 and name N)	4.60	0.08	0.07
	assign (segid 3A4 and resid 20 and name C)	(segid 3A4 and resid 22 and name O)	6.96	0.16	0.17
	assign (segid 3A4 and resid 20 and name C)	(segid 3A4 and resid 23 and name N)	7.67	0.14	0.15
	assign (segid 3A4 and resid 20 and name C)	(segid 3A4 and resid 31 and name C)	6.19	0.15	0.14
20	assign (segid 3A4 and resid 20 and name C)	(segid 3A4 and resid 31 and name CA)	6.21	0.14	0.15
	assign (segid 3A4 and resid 20 and name C)	(segid 3A4 and resid 31 and name CB)	6.05	0.13	0.13
	assign (segid 3A4 and resid 20 and name C)	(segid 3A4 and resid 31 and name N)	7.61	0.15	0.15
	assign (segid 3A4 and resid 20 and name C)	(segid 3A4 and resid 31 and name O)	7.21	0.20	0.20
	assign (segid 3A4 and resid 20 and name C)	(segid 3A4 and resid 32 and name C)	4.99	0.19	0.20
25	assign (segid 3A4 and resid 20 and name C)	(segid 3A4 and resid 32 and name CA)	5.77	0.14	0.14
	assign (segid 3A4 and resid 20 and name C)	(segid 3A4 and resid 32 and name CB)	6.15	0.17	0.17
	assign (segid 3A4 and resid 20 and name C)	(segid 3A4 and resid 32 and name N)	5.33	0.12	0.12
	assign (segid 3A4 and resid 20 and name C)	(segid 3A4 and resid 32 and name O)	3.86	0.26	0.25
	assign (segid 3A4 and resid 20 and name C)	(segid 3A4 and resid 33 and name C)	6.64	0.26	0.26
30	assign (segid 3A4 and resid 20 and name C)	(segid 3A4 and resid 33 and name CA)	5.83	0.26	0.26
	assign (segid 3A4 and resid 20 and name C)	(segid 3A4 and resid 33 and name CB)	6.80	0.33	0.33
	assign (segid 3A4 and resid 20 and name C)	(segid 3A4 and resid 33 and name N)	5.84	0.21	0.21
	assign (segid 3A4 and resid 20 and name C)	(segid 3A4 and resid 34 and name CA)	7.40	0.24	0.24
	assign (segid 3A4 and resid 20 and name C)	(segid 3A4 and resid 34 and name CB)	7.04	0.30	0.30
35	assign (segid 3A4 and resid 20 and name C)	(segid 3A4 and resid 34 and name N)	6.37	0.23	0.23
	assign (segid 3A4 and resid 20 and name C)	(segid 3A4 and resid 20 and name C)	1.51	0.00	0.00
	assign (segid 3A4 and resid 20 and name CA)	(segid 3A4 and resid 20 and name CB)	1.55	0.01	0.01
	assign (segid 3A4 and resid 20 and name CA)	(segid 3A4 and resid 20 and name O)	2.38	0.02	0.02
	assign (segid 3A4 and resid 20 and name CA)	(segid 3A4 and resid 21 and name C)	4.72	0.05	0.06
40	assign (segid 3A4 and resid 20 and name CA)	(segid 3A4 and resid 21 and name CA)	3.77	0.03	0.02
	assign (segid 3A4 and resid 20 and name CA)	(segid 3A4 and resid 21 and name CB)	4.55	0.07	0.08
	assign (segid 3A4 and resid 20 and name CA)	(segid 3A4 and resid 21 and name N)	2.42	0.02	0.01
	assign (segid 3A4 and resid 20 and name CA)	(segid 3A4 and resid 21 and name O)	4.68	0.14	0.14
	assign (segid 3A4 and resid 20 and name CA)	(segid 3A4 and resid 22 and name CA)	7.03	0.08	0.09
45	assign (segid 3A4 and resid 20 and name CA)	(segid 3A4 and resid 22 and name N)	5.88	0.08	0.08
	assign (segid 3A4 and resid 20 and name CA)	(segid 3A4 and resid 23 and name CA)	9.85	0.18	0.19
	assign (segid 3A4 and resid 20 and name CA)	(segid 3A4 and resid 23 and name CB)	9.87	0.29	0.29
	assign (segid 3A4 and resid 20 and name CA)	(segid 3A4 and resid 24 and name CA)	13.40	0.18	0.18
	assign (segid 3A4 and resid 20 and name CA)	(segid 3A4 and resid 24 and name CB)	14.12	0.37	0.37
50	assign (segid 3A4 and resid 20 and name CA)	(segid 3A4 and resid 25 and name CA)	15.68	0.41	0.40
	assign (segid 3A4 and resid 20 and name CA)	(segid 3A4 and resid 26 and name CA)	18.84	0.88	0.89
	assign (segid 3A4 and resid 20 and name CA)	(segid 3A4 and resid 29 and name CA)	12.88	0.17	0.17
	assign (segid 3A4 and resid 20 and name CA)	(segid 3A4 and resid 30 and name CA)	10.24	0.20	0.19
	assign (segid 3A4 and resid 20 and name CA)	(segid 3A4 and resid 31 and name C)	6.30	0.20	0.20
55	assign (segid 3A4 and resid 20 and name CA)	(segid 3A4 and resid 31 and name CB)	6.57	0.17	0.17
	assign (segid 3A4 and resid 20 and name CA)	(segid 3A4 and resid 31 and name O)	6.26	0.13	0.14
	assign (segid 3A4 and resid 20 and name CA)	(segid 3A4 and resid 31 and name N)	7.15	0.29	0.28
	assign (segid 3A4 and resid 20 and name CA)	(segid 3A4 and resid 322 and name CA)	14.07	0.61	0.62
	assign (segid 3A4 and resid 20 and name CA)	(segid 3A4 and resid 323 and name CA)	14.04	0.27	0.27
60	assign (segid 3A4 and resid 20 and name CA)	(segid 3A4 and resid 323 and name CB)	13.37	0.33	0.33
	assign (segid 3A4 and resid 20 and name CA)	(segid 3A4 and resid 324 and name CA)	14.80	0.10	0.09
	assign (segid 3A4 and resid 20 and name CA)	(segid 3A4 and resid 324 and name CB)	16.15	0.13	0.14
	assign (segid 3A4 and resid 20 and name CA)	(segid 3A4 and resid 325 and name CA)	14.43	0.32	0.32
	assign (segid 3A4 and resid 20 and name CA)	(segid 3A4 and resid 325 and name CB)	13.52	0.43	0.43
65	assign (segid 3A4 and resid 20 and name CA)	(segid 3A4 and resid 326 and name CA)	18.03	0.37	0.36
	assign (segid 3A4 and resid 20 and name CA)	(segid 3A4 and resid 326 and name CB)	18.86	0.33	0.32
	assign (segid 3A4 and resid 20 and name CA)	(segid 3A4 and resid 327 and name CA)	17.77	0.70	0.71
	assign (segid 3A4 and resid 20 and name CA)	(segid 3A4 and resid 328 and name CA)	15.66	0.91	0.90
	assign (segid 3A4 and resid 20 and name CA)	(segid 3A4 and resid 328 and name CB)	16.34	1.00	1.00
70	assign (segid 3A4 and resid 20 and name CA)	(segid 3A4 and resid 329 and name CA)	13.35	0.99	0.99
	assign (segid 3A4 and resid 20 and name CA)	(segid 3A4 and resid 329 and name CB)	13.07	1.01	1.00
	assign (segid 3A4 and resid 20 and name CA)	(segid 3A4 and resid 32 and name C)	4.52	0.17	0.17
	assign (segid 3A4 and resid 20 and name CA)	(segid 3A4 and resid 32 and name CA)	5.62	0.15	0.15
	assign (segid 3A4 and resid 20 and name CA)	(segid 3A4 and resid 32 and name CB)	6.19	0.17	0.16
75	assign (segid 3A4 and resid 20 and name CA)	(segid 3A4 and resid 32 and name N)	5.44	0.16	0.16
	assign (segid 3A4 and resid 20 and name CA)	(segid 3A4 and resid 32 and name O)	3.43	0.18	0.18
	assign (segid 3A4 and resid 20 and name CA)	(segid 3A4 and resid 330 and name CA)	11.37	0.95	0.95
	assign (segid 3A4 and resid 20 and name CA)	(segid 3A4 and resid 330 and name CB)	12.31	0.95	0.96
	assign (segid 3A4 and resid 20 and name CA)	(segid 3A4 and resid 331 and name CA)	8.57	0.90	0.91
80	assign (segid 3A4 and resid 20 and name CA)	(segid 3A4 and resid 331 and name CB)	7.75	0.79	0.80
	assign (segid 3A4 and resid 20 and name CA)	(segid 3A4 and resid 332 and name CA)	8.24	1.14	1.13
	assign (segid 3A4 and resid 20 and name CA)	(segid 3A4 and resid 333 and name CA)	9.83	1.44	1.44

	assign	(segid 3A4 and resid 20 and name CA)	(segid 3A4 and resid 335 and name CA)	7.88	0.83	0.82
	assign	(segid 3A4 and resid 20 and name CA)	(segid 3A4 and resid 336 and name CA)	10.53	0.78	0.77
	assign	(segid 3A4 and resid 20 and name CA)	(segid 3A4 and resid 337 and name CB)	11.76	0.72	0.72
	assign	(segid 3A4 and resid 20 and name CA)	(segid 3A4 and resid 337 and name CA)	10.45	0.92	0.93
5	assign	(segid 3A4 and resid 20 and name CA)	(segid 3A4 and resid 337 and name CB)	9.88	0.88	0.89
	assign	(segid 3A4 and resid 20 and name CA)	(segid 3A4 and resid 338 and name CA)	13.94	0.87	0.87
	assign	(segid 3A4 and resid 20 and name CA)	(segid 3A4 and resid 338 and name CB)	14.47	0.93	0.93
	assign	(segid 3A4 and resid 20 and name CA)	(segid 3A4 and resid 339 and name CA)	16.42	0.72	0.72
	assign	(segid 3A4 and resid 20 and name CA)	(segid 3A4 and resid 339 and name CB)	17.86	0.76	0.76
10	assign	(segid 3A4 and resid 20 and name CA)	(segid 3A4 and resid 33 and name C)	5.57	0.21	0.22
	assign	(segid 3A4 and resid 20 and name CA)	(segid 3A4 and resid 33 and name CA)	4.76	0.24	0.23
	assign	(segid 3A4 and resid 20 and name CA)	(segid 3A4 and resid 33 and name CB)	5.62	0.34	0.34
	assign	(segid 3A4 and resid 20 and name CA)	(segid 3A4 and resid 33 and name N)	5.08	0.18	0.19
	assign	(segid 3A4 and resid 20 and name CA)	(segid 3A4 and resid 33 and name O)	6.73	0.24	0.24
15	assign	(segid 3A4 and resid 20 and name CA)	(segid 3A4 and resid 340 and name CA)	16.64	0.31	0.31
	assign	(segid 3A4 and resid 20 and name CA)	(segid 3A4 and resid 341 and name CA)	13.17	0.28	0.27
	assign	(segid 3A4 and resid 20 and name CA)	(segid 3A4 and resid 341 and name CB)	12.03	0.36	0.35
	assign	(segid 3A4 and resid 20 and name CA)	(segid 3A4 and resid 342 and name CA)	12.39	0.19	0.19
	assign	(segid 3A4 and resid 20 and name CA)	(segid 3A4 and resid 343 and name CA)	9.56	0.28	0.29
20	assign	(segid 3A4 and resid 20 and name CA)	(segid 3A4 and resid 343 and name CB)	9.27	0.38	0.38
	assign	(segid 3A4 and resid 20 and name CA)	(segid 3A4 and resid 344 and name CA)	9.88	0.27	0.28
	assign	(segid 3A4 and resid 20 and name CA)	(segid 3A4 and resid 344 and name CB)	10.09	0.38	0.39
	assign	(segid 3A4 and resid 20 and name CA)	(segid 3A4 and resid 345 and name CA)	9.70	0.34	0.33
	assign	(segid 3A4 and resid 20 and name CA)	(segid 3A4 and resid 345 and name CB)	10.49	0.40	0.39
25	assign	(segid 3A4 and resid 20 and name CA)	(segid 3A4 and resid 346 and name CA)	10.64	0.50	0.49
	assign	(segid 3A4 and resid 20 and name CA)	(segid 3A4 and resid 346 and name CB)	9.95	0.57	0.57
	assign	(segid 3A4 and resid 20 and name CA)	(segid 3A4 and resid 347 and name CA)	13.50	0.49	0.49
	assign	(segid 3A4 and resid 20 and name CA)	(segid 3A4 and resid 347 and name CB)	14.79	0.50	0.50
	assign	(segid 3A4 and resid 20 and name CA)	(segid 3A4 and resid 348 and name CA)	14.70	0.39	0.39
30	assign	(segid 3A4 and resid 20 and name CA)	(segid 3A4 and resid 349 and name CA)	11.86	0.46	0.46
	assign	(segid 3A4 and resid 20 and name CA)	(segid 3A4 and resid 349 and name CB)	10.45	0.42	0.42
	assign	(segid 3A4 and resid 20 and name CA)	(segid 3A4 and resid 34 and name C)	7.14	0.13	0.12
	assign	(segid 3A4 and resid 20 and name CA)	(segid 3A4 and resid 34 and name CA)	6.36	0.15	0.16
	assign	(segid 3A4 and resid 20 and name CA)	(segid 3A4 and resid 34 and name CB)	6.22	0.25	0.24
35	assign	(segid 3A4 and resid 20 and name CA)	(segid 3A4 and resid 34 and name N)	5.26	0.16	0.16
	assign	(segid 3A4 and resid 20 and name CA)	(segid 3A4 and resid 350 and name CA)	12.34	0.81	0.81
	assign	(segid 3A4 and resid 20 and name CA)	(segid 3A4 and resid 350 and name CB)	12.49	0.90	0.89
	assign	(segid 3A4 and resid 20 and name CA)	(segid 3A4 and resid 351 and name CA)	15.97	0.72	0.72
	assign	(segid 3A4 and resid 20 and name CA)	(segid 3A4 and resid 352 and name CA)	15.66	0.81	0.82
40	assign	(segid 3A4 and resid 20 and name CA)	(segid 3A4 and resid 352 and name CB)	15.58	0.85	0.86
	assign	(segid 3A4 and resid 20 and name CA)	(segid 3A4 and resid 353 and name CA)	13.79	0.92	0.92
	assign	(segid 3A4 and resid 20 and name CA)	(segid 3A4 and resid 353 and name CB)	13.10	1.00	1.00
	assign	(segid 3A4 and resid 20 and name CA)	(segid 3A4 and resid 354 and name CA)	16.33	0.93	0.93
	assign	(segid 3A4 and resid 20 and name CA)	(segid 3A4 and resid 354 and name CB)	16.41	0.92	0.92
45	assign	(segid 3A4 and resid 20 and name CA)	(segid 3A4 and resid 355 and name CA)	16.10	1.27	1.27
	assign	(segid 3A4 and resid 20 and name CA)	(segid 3A4 and resid 355 and name CB)	15.02	1.38	1.38
	assign	(segid 3A4 and resid 20 and name CA)	(segid 3A4 and resid 356 and name CB)	16.57	0.92	0.92
	assign	(segid 3A4 and resid 20 and name CA)	(segid 3A4 and resid 35 and name CA)	7.85	0.24	0.24
	assign</					

	assign (segid 3A4 and resid 20 and name CB) (segid 3A4 and resid 322 and name CA)	14.12	0.68	0.68
	assign (segid 3A4 and resid 20 and name CB) (segid 3A4 and resid 323 and name CA)	13.70	0.33	0.32
	assign (segid 3A4 and resid 20 and name CB) (segid 3A4 and resid 323 and name CB)	12.93	0.36	0.36
	assign (segid 3A4 and resid 20 and name CB) (segid 3A4 and resid 324 and name CA)	14.25	0.10	0.10
	assign (segid 3A4 and resid 20 and name CB) (segid 3A4 and resid 324 and name CB)	15.64	0.11	0.11
5	assign (segid 3A4 and resid 20 and name CB) (segid 3A4 and resid 325 and name CA)	13.54	0.31	0.31
	assign (segid 3A4 and resid 20 and name CB) (segid 3A4 and resid 325 and name CB)	12.58	0.40	0.39
	assign (segid 3A4 and resid 20 and name CB) (segid 3A4 and resid 326 and name CA)	17.03	0.36	0.36
	assign (segid 3A4 and resid 20 and name CB) (segid 3A4 and resid 326 and name CB)	17.84	0.32	0.32
	assign (segid 3A4 and resid 20 and name CB) (segid 3A4 and resid 327 and name CA)	16.60	0.71	0.71
10	assign (segid 3A4 and resid 20 and name CB) (segid 3A4 and resid 327 and name CB)	17.29	0.79	0.80
	assign (segid 3A4 and resid 20 and name CB) (segid 3A4 and resid 328 and name CA)	14.40	0.90	0.90
	assign (segid 3A4 and resid 20 and name CB) (segid 3A4 and resid 328 and name CB)	15.07	0.99	0.99
	assign (segid 3A4 and resid 20 and name CB) (segid 3A4 and resid 329 and name CA)	11.96	0.98	0.97
	assign (segid 3A4 and resid 20 and name CB) (segid 3A4 and resid 329 and name CB)	11.71	0.99	0.98
15	assign (segid 3A4 and resid 20 and name CB) (segid 3A4 and resid 32 and name C)	5.26	0.16	0.16
	assign (segid 3A4 and resid 20 and name CB) (segid 3A4 and resid 32 and name CA)	6.38	0.17	0.16
	assign (segid 3A4 and resid 20 and name CB) (segid 3A4 and resid 32 and name CB)	7.21	0.17	0.18
	assign (segid 3A4 and resid 20 and name CB) (segid 3A4 and resid 32 and name N)	6.05	0.18	0.18
	assign (segid 3A4 and resid 20 and name CB) (segid 3A4 and resid 32 and name O)	4.37	0.18	0.18
20	assign (segid 3A4 and resid 20 and name CB) (segid 3A4 and resid 330 and name CA)	9.87	0.95	0.94
	assign (segid 3A4 and resid 20 and name CB) (segid 3A4 and resid 330 and name CB)	10.81	0.95	0.94
	assign (segid 3A4 and resid 20 and name CB) (segid 3A4 and resid 331 and name CA)	7.07	0.89	0.89
	assign (segid 3A4 and resid 20 and name CB) (segid 3A4 and resid 331 and name CB)	6.30	0.76	0.75
	assign (segid 3A4 and resid 20 and name CB) (segid 3A4 and resid 332 and name CA)	6.91	1.06	1.06
25	assign (segid 3A4 and resid 20 and name CB) (segid 3A4 and resid 332 and name CB)	8.56	1.33	1.33
	assign (segid 3A4 and resid 20 and name CB) (segid 3A4 and resid 333 and name CA)	6.62	0.76	0.77
	assign (segid 3A4 and resid 20 and name CB) (segid 3A4 and resid 335 and name CA)	9.26	0.78	0.77
	assign (segid 3A4 and resid 20 and name CB) (segid 3A4 and resid 336 and name CA)	10.53	0.71	0.72
	assign (segid 3A4 and resid 20 and name CB) (segid 3A4 and resid 336 and name CB)	9.35	0.89	0.90
30	assign (segid 3A4 and resid 20 and name CB) (segid 3A4 and resid 337 and name CA)	8.76	0.84	0.85
	assign (segid 3A4 and resid 20 and name CB) (segid 3A4 and resid 337 and name CB)	12.97	0.85	0.84
	assign (segid 3A4 and resid 20 and name CB) (segid 3A4 and resid 338 and name CA)	13.59	0.89	0.90
	assign (segid 3A4 and resid 20 and name CB) (segid 3A4 and resid 338 and name CB)	15.46	0.73	0.73
	assign (segid 3A4 and resid 20 and name CB) (segid 3A4 and resid 339 and name CA)	16.87	0.77	0.77
35	assign (segid 3A4 and resid 20 and name CB) (segid 3A4 and resid 339 and name CB)	6.20	0.15	0.15
	assign (segid 3A4 and resid 20 and name CB) (segid 3A4 and resid 33 and name C)	5.17	0.16	0.16
	assign (segid 3A4 and resid 20 and name CB) (segid 3A4 and resid 33 and name CA)	5.64	0.27	0.26
	assign (segid 3A4 and resid 20 and name CB) (segid 3A4 and resid 33 and name CB)	5.62	0.16	0.16
	assign (segid 3A4 and resid 20 and name CB) (segid 3A4 and resid 33 and name N)	7.36	0.17	0.16
40	assign (segid 3A4 and resid 20 and name CB) (segid 3A4 and resid 33 and name O)	15.96	0.33	0.33
	assign (segid 3A4 and resid 20 and name CB) (segid 3A4 and resid 340 and name CA)	12.64	0.26	0.26
	assign (segid 3A4 and resid 20 and name CB) (segid 3A4 and resid 341 and name CA)	11.44	0.33	0.33
	assign (segid 3A4 and resid 20 and name CB) (segid 3A4 and resid 341 and name CB)	12.16	0.25	0.26
	assign (segid 3A4 and resid 20 and name CB) (segid 3A4 and resid 342 and name CA)	9.40	0.33	0.34
45	assign (segid 3A4 and resid 20 and name CB) (segid 3A4 and resid 343 and name CA)	8.90	0.42	0.43
	assign (segid 3A4 and resid 20 and name CB) (segid 3A4 and resid 344 and name CA)	10.20	0.29	0.29
	assign (segid 3A4 and resid 20 and name CB) (segid 3A4 and resid 344 and name CB)	10.60	0.40	0.40
	assign (segid 3A4 and resid 20 and name CB) (segid 3A4 and resid 345 and name CA)	9.97	0.27	0.26
	assign (segid 3A4 and resid 20 and name CB) (segid 3A4 and resid 345 and name CB)	10.57	0.34	0.35
50	assign (segid 3A4 and resid 20 and name CB) (segid 3A4 and resid 346 and name CA)	11.34	0.40	0.40
	assign (segid 3A4 and resid 20 and name CB) (segid 3A4 and resid 346 and name CB)	10.83	0.50	0.49
	assign (segid 3A4 and resid 20 and name CB) (segid 3A4 and resid 347 and name CA)	14.03	0.40	0.41
	assign (segid 3A4 and resid 20 and name CB) (segid 3A4 and resid 347 and name CB)	15.26	0.41	0.41
	assign (segid 3A4 and resid 20 and name CB) (segid 3A4 and resid 348 and name CA)	15.55	0.34	0.34
55	assign (segid 3A4 and resid 20 and name CB) (segid 3A4 and resid 349 and name CA)	12.78	0.44	0.45
	assign (segid 3A4 and resid 20 and name CB) (segid 3A4 and resid 349 and name CB)	11.43	0.40	0.40
	assign (segid 3A4 and resid 20 and name CB) (segid 3A4 and resid 34 and name CA)	7.22	0.17	0.17
	assign (segid 3A4 and resid 20 and name CB) (segid 3A4 and resid 34 and name CB)	7.32	0.28	0.28
	assign (segid 3A4 and resid 20 and name CB) (segid 3A4 and resid 34 and name N)	6.00	0.15	0.16
60	assign (segid 3A4 and resid 20 and name CB) (segid 3A4 and resid 350 and name CA)	12.88	0.82	0.82
	assign (segid 3A4 and resid 20 and name CB) (segid 3A4 and resid 350 and name CB)	12.89	0.90	0.89
	assign (segid 3A4 and resid 20 and name CB) (segid 3A4 and resid 351 and name CA)	16.57	0.74	0.75
	assign (segid 3A4 and resid 20 and name CB) (segid 3A4 and resid 352 and name CA)	16.50	0.85	0.85
	assign (segid 3A4 and resid 20 and name CB) (segid 3A4 and resid 352 and name CB)	16.53	0.87	0.87
65	assign (segid 3A4 and resid 20 and name CB) (segid 3A4 and resid 353 and name CA)	14.45	0.99	1.00
	assign (segid 3A4 and resid 20 and name CB) (segid 3A4 and resid 353 and name CB)	13.63	1.09	1.08
	assign (segid 3A4 and resid 20 and name CB) (segid 3A4 and resid 354 and name CA)	16.99	1.04	1.04
	assign (segid 3A4 and resid 20 and name CB) (segid 3A4 and resid 354 and name CB)	17.13	1.04	1.04
	assign (segid 3A4 and resid 20 and name CB) (segid 3A4 and resid 355 and name CA)	15.26	1.51	1.51
70	assign (segid 3A4 and resid 20 and name CB) (segid 3A4 and resid 356 and name CB)	16.81	1.01	1.01
	assign (segid 3A4 and resid 20 and name CB) (segid 3A4 and resid 35 and name CA)	8.21	0.29	0.28
	assign (segid 3A4 and resid 20 and name CB) (segid 3A4 and resid 35 and name N)	7.28	0.22	0.23
	assign (segid 3A4 and resid 20 and name CB) (segid 3A4 and resid 36 and name CA)	11.12	0.22	0.22
75	assign (segid 3A4 and resid 20 and name CB) (segid 3A4 and resid 37 and name CA)	10.42	0.25	0.25
	assign (segid 3A4 and resid 20 and name CB) (segid 3A4 and resid 37 and name CB)	10.35	0.30	0.29
	assign (segid 3A4 and resid 20 and name CB) (segid 3A4 and resid 382 and name CA)	17.63	0.54	0.53
	assign (segid 3A4 and resid 20 and name CB) (segid 3A4 and resid 382 and name CB)	16.16	0.51	0.54
	assign (segid 3A4 and resid 20 and name CB) (segid 3A4 and resid 385 and name CA)	18.23	0.37	0.36
80	assign (segid 3A4 and resid 20 and name CB) (segid 3A4 and resid 386 and name CA)	17.86	0.35	0.36
	assign (segid 3A4 and resid 20 and name CB) (segid 3A4 and resid 38 and name CA)	7.33	0.30	0.30
	assign (segid 3A4 and resid 20 and name CB) (segid 3A4 and resid 38 and name CB)	5.93	0.21	0.22
	assign (segid 3A4 and resid 20 and name CB) (segid 3A4 and resid 39 and name CA)	9.42	0.30	0.30

	assign (segid 3A4 and resid 20 and name CB)	(segid 3A4 and resid 39 and name CB)	10.06	0.33	0.32
	assign (segid 3A4 and resid 20 and name CB)	(segid 3A4 and resid 40 and name CA)	12.45	0.28	0.27
	assign (segid 3A4 and resid 20 and name CB)	(segid 3A4 and resid 40 and name CB)	13.19	0.25	0.24
	assign (segid 3A4 and resid 20 and name CB)	(segid 3A4 and resid 41 and name CA)	11.22	0.33	0.33
5	assign (segid 3A4 and resid 20 and name CB)	(segid 3A4 and resid 41 and name CB)	10.23	0.33	0.33
	assign (segid 3A4 and resid 20 and name CB)	(segid 3A4 and resid 42 and name CA)	10.33	0.43	0.43
	assign (segid 3A4 and resid 20 and name CB)	(segid 3A4 and resid 42 and name CB)	9.30	0.44	0.43
	assign (segid 3A4 and resid 20 and name CB)	(segid 3A4 and resid 20 and name C)	2.36	0.04	0.05
	assign (segid 3A4 and resid 20 and name N)	(segid 3A4 and resid 20 and name CA)	1.46	0.01	0.01
	assign (segid 3A4 and resid 20 and name N)	(segid 3A4 and resid 20 and name CB)	2.47	0.03	0.03
10	assign (segid 3A4 and resid 20 and name N)	(segid 3A4 and resid 20 and name O)	2.83	0.08	0.08
	assign (segid 3A4 and resid 20 and name N)	(segid 3A4 and resid 21 and name C)	5.72	0.06	0.06
	assign (segid 3A4 and resid 20 and name N)	(segid 3A4 and resid 21 and name CA)	4.54	0.08	0.08
	assign (segid 3A4 and resid 20 and name N)	(segid 3A4 and resid 21 and name CB)	4.93	0.14	0.15
	assign (segid 3A4 and resid 20 and name N)	(segid 3A4 and resid 21 and name N)	3.32	0.08	0.08
15	assign (segid 3A4 and resid 20 and name N)	(segid 3A4 and resid 21 and name O)	5.80	0.11	0.11
	assign (segid 3A4 and resid 20 and name N)	(segid 3A4 and resid 22 and name N)	6.84	0.06	0.06
	assign (segid 3A4 and resid 20 and name N)	(segid 3A4 and resid 31 and name C)	7.57	0.22	0.22
	assign (segid 3A4 and resid 20 and name N)	(segid 3A4 and resid 31 and name CB)	7.71	0.15	0.14
	assign (segid 3A4 and resid 20 and name N)	(segid 3A4 and resid 32 and name C)	5.37	0.19	0.19
20	assign (segid 3A4 and resid 20 and name N)	(segid 3A4 and resid 32 and name CA)	6.57	0.17	0.17
	assign (segid 3A4 and resid 20 and name N)	(segid 3A4 and resid 32 and name CB)	6.93	0.18	0.19
	assign (segid 3A4 and resid 20 and name N)	(segid 3A4 and resid 32 and name N)	6.60	0.17	0.17
	assign (segid 3A4 and resid 20 and name N)	(segid 3A4 and resid 32 and name O)	4.25	0.19	0.19
	assign (segid 3A4 and resid 20 and name N)	(segid 3A4 and resid 33 and name C)	5.76	0.29	0.29
25	assign (segid 3A4 and resid 20 and name N)	(segid 3A4 and resid 33 and name CA)	5.28	0.29	0.29
	assign (segid 3A4 and resid 20 and name N)	(segid 3A4 and resid 33 and name CB)	6.20	0.39	0.38
	assign (segid 3A4 and resid 20 and name N)	(segid 3A4 and resid 33 and name N)	5.83	0.22	0.22
	assign (segid 3A4 and resid 20 and name N)	(segid 3A4 and resid 33 and name O)	6.94	0.30	0.31
	assign (segid 3A4 and resid 20 and name N)	(segid 3A4 and resid 34 and name C)	6.58	0.21	0.21
30	assign (segid 3A4 and resid 20 and name N)	(segid 3A4 and resid 34 and name CA)	5.99	0.22	0.22
	assign (segid 3A4 and resid 20 and name N)	(segid 3A4 and resid 34 and name CB)	5.67	0.28	0.27
	assign (segid 3A4 and resid 20 and name N)	(segid 3A4 and resid 34 and name N)	5.12	0.24	0.24
	assign (segid 3A4 and resid 20 and name N)	(segid 3A4 and resid 35 and name CA)	7.12	0.31	0.31
	assign (segid 3A4 and resid 20 and name N)	(segid 3A4 and resid 35 and name N)	6.17	0.29	0.30
35	assign (segid 3A4 and resid 20 and name N)	(segid 3A4 and resid 38 and name CB)	6.40	0.56	0.56
	assign (segid 3A4 and resid 20 and name O)	(segid 3A4 and resid 20 and name CB)	2.96	0.11	0.11
	assign (segid 3A4 and resid 20 and name O)	(segid 3A4 and resid 21 and name C)	4.04	0.03	0.03
	assign (segid 3A4 and resid 20 and name O)	(segid 3A4 and resid 21 and name CA)	2.75	0.07	0.07
40	assign (segid 3A4 and resid 20 and name O)	(segid 3A4 and resid 21 and name CB)	3.52	0.23	0.24
	assign (segid 3A4 and resid 20 and name O)	(segid 3A4 and resid 21 and name N)	2.25	0.03	0.02
	assign (segid 3A4 and resid 20 and name O)	(segid 3A4 and resid 21 and name O)	4.59	0.09	0.08
	assign (segid 3A4 and resid 20 and name O)	(segid 3A4 and resid 22 and name C)	7.15	0.15	0.14
	assign (segid 3A4 and resid 20 and name O)	(segid 3A4 and resid 22 and name CA)	6.18	0.10	0.10
	assign (segid 3A4 and resid 20 and name O)	(segid 3A4 and resid 22 and name N)	4.83	0.11	0.11
45	assign (segid 3A4 and resid 20 and name O)	(segid 3A4 and resid 22 and name O)	7.20	0.21	0.20
	assign (segid 3A4 and resid 20 and name O)	(segid 3A4 and resid 31 and name C)	7.19	0.12	0.12
	assign (segid 3A4 and resid 20 and name O)	(segid 3A4 and resid 31 and name CA)	7.03	0.14	0.14
	assign (segid 3A4 and resid 20 and name O)	(segid 3A4 and resid 31 and name CB)	6.78	0.15	0.16
	assign (segid 3A4 and resid 20 and name O)	(segid 3A4 and resid 32 and name C)	6.20	0.20	0.21
50	assign (segid 3A4 and resid 20 and name O)	(segid 3A4 and resid 32 and name CA)	6.94	0.16	0.16
	assign (segid 3A4 and resid 20 and name O)	(segid 3A4 and resid 32 and name CB)	7.27	0.22	0.22
	assign (segid 3A4 and resid 20 and name O)	(segid 3A4 and resid 32 and name N)	6.40	0.10	0.10
	assign (segid 3A4 and resid 20 and name O)	(segid 3A4 and resid 32 and name O)	5.07	0.26	0.27
	assign (segid 3A4 and resid 20 and name O)	(segid 3A4 and resid 33 and name CA)	6.97	0.24	0.24
55	assign (segid 3A4 and resid 20 and name O)	(segid 3A4 and resid 33 and name N)	7.04	0.20	0.20
	assign (segid 3A4 and resid 20 and name O)	(segid 3A4 and resid 34 and name N)	7.41	0.23	0.24
	assign (segid 3A4 and resid 219 and name C)	(segid 3A4 and resid 219 and name CB)	2.52	0.02	0.03
	assign (segid 3A4 and resid 219 and name C)	(segid 3A4 and resid 219 and name CG)	3.09	0.09	0.09
60	assign (segid 3A4 and resid 219 and name C)	(segid 3A4 and resid 219 and name O)	1.24	0.01	0.00
	assign (segid 3A4 and resid 219 and name C)	(segid 3A4 and resid 220 and name C)	3.04	0.04	0.05
	assign (segid 3A4 and resid 219 and name C)	(segid 3A4 and resid 220 and name CA)	2.43	0.03	0.02
	assign (segid 3A4 and resid 219 and name C)	(segid 3A4 and resid 220 and name CB)	3.70	0.03	0.03
	assign (segid 3A4 and resid 219 and name C)	(segid 3A4 and resid 220 and name N)	1.32	0.00	0.01
	assign (segid 3A4 and resid 219 and name C)	(segid 3A4 and resid 220 and name O)	3.88	0.10	0.11
65	assign (segid 3A4 and resid 219 and name C)	(segid 3A4 and resid 221 and name C)	4.67	0.07	0.08
	assign (segid 3A4 and resid 219 and name C)	(segid 3A4 and resid 221 and name CA)	4.53	0.04	0.03
	assign (segid 3A4 and resid 219 and name C)	(segid 3A4 and resid 221 and name CB)	5.27	0.07	0.07
	assign (segid 3A4 and resid 219 and name C)	(segid 3A4 and resid 221 and name N)	3.32	0.02	0.03
	assign (segid 3A4 and resid 219 and name C)	(segid 3A4 and resid 221 and name O)	5.73	0.12	0.11
70	assign (segid 3A4 and resid 219 and name C)	(segid 3A4 and resid 222 and name C)	5.12	0.11	0.12
	assign (segid 3A4 and resid 219 and name C)	(segid 3A4 and resid 222 and name CA)	4.79	0.11	0.12
	assign (segid 3A4 and resid 219 and name C)	(segid 3A4 and resid 222 and name CB)	4.59	0.21	0.22
	assign (segid 3A4 and resid 219 and name C)	(segid 3A4 and resid 222 and name N)	4.02	0.05	0.04
	assign (segid 3A4 and resid 219 and name C)	(segid 3A4 and resid 222 and name O)	6.34	0.12	0.12
75	assign (segid 3A4 and resid 219 and name C)	(segid 3A4 and resid 223 and name C)	6.30	0.10	0.11
	assign (segid 3A4 and resid 219 and name C)	(segid 3A4 and resid 223 and name CA)	5.24	0.14	0.14
	assign (segid 3A4 and resid 219 and name C)	(segid 3A4 and resid 223 and name CB)	4.80	0.19	0.19
	assign (segid 3A4 and resid 219 and name C)	(segid 3A4 and resid 223 and name N)	4.37	0.13	0.13
80	assign (segid 3A4 and resid 219 and name C)	(segid 3A4 and resid 223 and name O)	7.46	0.11	0.10
	assign (segid 3A4 and resid 219 and name C)	(segid 3A4 and resid 224 and name CA)	7.45	0.10	0.10
	assign (segid 3A4 and resid 219 and name C)	(segid 3A4 and resid 224 and name CB)	7.49	0.11	0.10
	assign (segid 3A4 and resid 219 and name C)	(segid 3A4 and resid 224 and name N)	6.17	0.11	0.11

	assign (segid 3A4 and resid 219 and name CA)	(segid 3A4 and resid 219 and name C)	1.52	0.00	0.01
	assign (segid 3A4 and resid 219 and name CA)	(segid 3A4 and resid 219 and name CB)	1.53	0.01	0.01
	assign (segid 3A4 and resid 219 and name CA)	(segid 3A4 and resid 219 and name CG)	2.57	0.05	0.04
	assign (segid 3A4 and resid 219 and name CA)	(segid 3A4 and resid 219 and name O)	2.40	0.00	0.01
	assign (segid 3A4 and resid 219 and name CA)	(segid 3A4 and resid 220 and name C)	4.46	0.03	0.04
5	assign (segid 3A4 and resid 219 and name CA)	(segid 3A4 and resid 220 and name CA)	3.81	0.02	0.01
	assign (segid 3A4 and resid 219 and name CA)	(segid 3A4 and resid 220 and name CB)	4.85	0.02	0.03
	assign (segid 3A4 and resid 219 and name CA)	(segid 3A4 and resid 220 and name N)	2.44	0.02	0.01
	assign (segid 3A4 and resid 219 and name CA)	(segid 3A4 and resid 220 and name O)	5.37	0.10	0.09
	assign (segid 3A4 and resid 219 and name CA)	(segid 3A4 and resid 221 and name C)	5.74	0.03	0.03
10	assign (segid 3A4 and resid 219 and name CA)	(segid 3A4 and resid 221 and name CA)	5.61	0.05	0.05
	assign (segid 3A4 and resid 219 and name CA)	(segid 3A4 and resid 221 and name CB)	6.04	0.08	0.08
	assign (segid 3A4 and resid 219 and name CA)	(segid 3A4 and resid 221 and name N)	4.49	0.07	0.07
	assign (segid 3A4 and resid 219 and name CA)	(segid 3A4 and resid 221 and name O)	6.86	0.07	0.06
	assign (segid 3A4 and resid 219 and name CA)	(segid 3A4 and resid 222 and name C)	6.09	0.13	0.14
15	assign (segid 3A4 and resid 219 and name CA)	(segid 3A4 and resid 222 and name CA)	5.55	0.11	0.11
	assign (segid 3A4 and resid 219 and name CA)	(segid 3A4 and resid 222 and name CB)	4.98	0.23	0.23
	assign (segid 3A4 and resid 219 and name CA)	(segid 3A4 and resid 222 and name N)	4.91	0.03	0.02
	assign (segid 3A4 and resid 219 and name CA)	(segid 3A4 and resid 222 and name O)	7.29	0.15	0.14
	assign (segid 3A4 and resid 219 and name CA)	(segid 3A4 and resid 223 and name C)	7.63	0.14	0.13
20	assign (segid 3A4 and resid 219 and name CA)	(segid 3A4 and resid 223 and name CA)	6.45	0.18	0.18
	assign (segid 3A4 and resid 219 and name CA)	(segid 3A4 and resid 223 and name CB)	6.07	0.23	0.23
	assign (segid 3A4 and resid 219 and name CA)	(segid 3A4 and resid 223 and name N)	5.51	0.14	0.15
	assign (segid 3A4 and resid 219 and name CA)	(segid 3A4 and resid 224 and name CA)	8.88	0.09	0.09
	assign (segid 3A4 and resid 219 and name CA)	(segid 3A4 and resid 224 and name CB)	8.94	0.09	0.08
25	assign (segid 3A4 and resid 219 and name CA)	(segid 3A4 and resid 224 and name N)	7.58	0.11	0.10
	assign (segid 3A4 and resid 219 and name CA)	(segid 3A4 and resid 225 and name CA)	10.21	0.11	0.12
	assign (segid 3A4 and resid 219 and name CA)	(segid 3A4 and resid 225 and name CB)	9.76	0.15	0.14
	assign (segid 3A4 and resid 219 and name CA)	(segid 3A4 and resid 226 and name CA)	11.17	0.25	0.26
	assign (segid 3A4 and resid 219 and name CA)	(segid 3A4 and resid 240 and name CA)	17.93	0.60	0.59
30	assign (segid 3A4 and resid 219 and name CA)	(segid 3A4 and resid 241 and name CA)	16.54	0.66	0.65
	assign (segid 3A4 and resid 219 and name CA)	(segid 3A4 and resid 241 and name CB)	17.23	0.73	0.72
	assign (segid 3A4 and resid 219 and name CA)	(segid 3A4 and resid 242 and name CA)	18.28	0.59	0.60
	assign (segid 3A4 and resid 219 and name CA)	(segid 3A4 and resid 243 and name CA)	16.91	0.37	0.36
	assign (segid 3A4 and resid 219 and name CA)	(segid 3A4 and resid 243 and name CB)	17.18	0.34	0.34
35	assign (segid 3A4 and resid 219 and name CA)	(segid 3A4 and resid 244 and name CA)	13.28	0.43	0.43
	assign (segid 3A4 and resid 219 and name CA)	(segid 3A4 and resid 244 and name CB)	12.80	0.50	0.49
	assign (segid 3A4 and resid 219 and name CA)	(segid 3A4 and resid 245 and name CA)	14.36	0.43	0.43
	assign (segid 3A4 and resid 219 and name CA)	(segid 3A4 and resid 245 and name CB)	15.56	0.42	0.43
	assign (segid 3A4 and resid 219 and name CA)	(segid 3A4 and resid 246 and name CA)	16.29	0.35	0.34
40	assign (segid 3A4 and resid 219 and name CA)	(segid 3A4 and resid 246 and name CB)	17.47	0.39	0.39
	assign (segid 3A4 and resid 219 and name CA)	(segid 3A4 and resid 247 and name CA)	13.64	0.38	0.38
	assign (segid 3A4 and resid 219 and name CA)	(segid 3A4 and resid 247 and name CB)	12.95	0.44	0.44
	assign (segid 3A4 and resid 219 and name CA)	(segid 3A4 and resid 248 and name CA)	11.37	0.27	0.26
	assign (segid 3A4 and resid 219 and name CA)	(segid 3A4 and resid 248 and name CB)	10.94	0.33	0.34
45	assign (segid 3A4 and resid 219 and name CA)	(segid 3A4 and resid 249 and name CA)	14.67	0.26	0.27
	assign (segid 3A4 and resid 219 and name CA)	(segid 3A4 and resid 250 and name CA)	15.58	0.28	0.29
	assign (segid 3A4 and resid 219 and name CA)	(segid 3A4 and resid 250 and name CB)	15.93	0.42	0.42
	assign (segid 3A4 and resid 219 and name CA)	(segid 3A4 and resid 251 and name CA)	12.63	0.24	0.24
	assign (segid 3A4 and resid 219 and name CA)	(segid 3A4 and resid 251 and name CB)	11.19	0.24	0.24
50	assign (segid 3A4 and resid 219 and name CA)	(segid 3A4 and resid 252 and name CA)	13.39	0.37	0.37
	assign (segid 3A4 and resid 219 and name CA)	(segid 3A4 and resid 252 and name CB)	13.46	0.38	0.38
	assign (segid 3A4 and resid 219 and name CA)	(segid 3A4 and resid 253 and name CA)	17.08	0.33	0.34
	assign (segid 3A4 and resid 219 and name CA)	(segid 3A4 and resid 254 and name CA)	17.36	0.55	0.54
	assign (segid 3A4 and resid 219 and name CA)	(segid 3A4 and resid 255 and name CA)	15.53	1.18	1.19
55	assign (segid 3A4 and resid 219 and name CA)	(segid 3A4 and resid 256 and name CA)	17.00	0.46	0.45
	assign (segid 3A4 and resid 219 and name CA)	(segid 3A4 and resid 259 and name CB)	18.52	0.56	0.55
	assign (segid 3A4 and resid 219 and name CA)	(segid 3A4 and resid 392 and name CA)	16.31	0.62	0.62
	assign (segid 3A4 and resid 219 and name CA)	(segid 3A4 and resid 392 and name CB)	15.51	0.53	0.53
60	assign (segid 3A4 and resid 219 and name CA)	(segid 3A4 and resid 393 and name CA)	14.99	0.64	0.64
	assign (segid 3A4 and resid 219 and name CA)	(segid 3A4 and resid 394 and name CA)	18.16	0.71	0.72
	assign (segid 3A4 and resid 219 and name CA)	(segid 3A4 and resid 395 and name CA)	16.82	0.87	0.88
	assign (segid 3A4 and resid 219 and name CA)	(segid 3A4 and resid 396 and name CA)	14.34	0.93	0.92
	assign (segid 3A4 and resid 219 and name CA)	(segid 3A4 and resid 396 and name CB)	13.09	0.89	0.88
	assign (segid 3A4 and resid 219 and name CA)	(segid 3A4 and resid 397 and name CA)	17.24	0.89	0.89
65	assign (segid 3A4 and resid 219 and name CA)	(segid 3A4 and resid 397 and name CB)	18.00	0.84	0.84
	assign (segid 3A4 and resid 219 and name CA)	(segid 3A4 and resid 399 and name CA)	17.87	1.02	1.02
	assign (segid 3A4 and resid 219 and name CA)	(segid 3A4 and resid 399 and name CB)	16.58	1.02	1.01
	assign (segid 3A4 and resid 219 and name CA)	(segid 3A4 and resid 400 and name CA)	17.47	1.12	1.12
	assign (segid 3A4 and resid 219 and name CA)	(segid 3A4 and resid 400 and name CB)	16.75	1.14	1.13
70	assign (segid 3A4 and resid 219 and name CA)	(segid 3A4 and resid 219 and name CG)	1.52	0.01	0.01
	assign (segid 3A4 and resid 219 and name CB)	(segid 3A4 and resid 220 and name C)	4.84	0.06	0.07
	assign (segid 3A4 and resid 219 and name CB)	(segid 3A4 and resid 220 and name CA)	4.44	0.03	0.04
	assign (segid 3A4 and resid 219 and name CB)	(segid 3A4 and resid 220 and name CB)	5.30	0.11	0.11
	assign (segid 3A4 and resid 219 and name CB)	(segid 3A4 and resid 220 and name N)	3.09	0.04	0.04
75	assign (segid 3A4 and resid 219 and name CB)	(segid 3A4 and resid 220 and name O)	5.89	0.07	0.07
	assign (segid 3A4 and resid 219 and name CB)	(segid 3A4 and resid 221 and name C)	5.71	0.14	0.13
	assign (segid 3A4 and resid 219 and name CB)	(segid 3A4 and resid 221 and name CA)	5.41	0.16	0.15
	assign (segid 3A4 and resid 219 and name CB)	(segid 3A4 and resid 221 and name CB)	5.45	0.18	0.17
	assign (segid 3A4 and resid 219 and name CB)	(segid 3A4 and resid 221 and name N)	4.45	0.14	0.13
80	assign (segid 3A4 and resid 219 and name CB)	(segid 3A4 and resid 221 and name O)	6.91	0.12	0.11
	assign (segid 3A4 and resid 219 and name CB)	(segid 3A4 and resid 222 and name C)	6.59	0.11	0.11
	assign (segid 3A4 and resid 219 and name CB)	(segid 3A4 and resid 222 and name CA)	5.72	0.13	0.14

	assign (segid 3A4 and resid 219 and name CB)	(segid 3A4 and resid 222 and name CB)	5.18	0.22	0.23
	assign (segid 3A4 and resid 219 and name CB)	(segid 3A4 and resid 222 and name N)	4.92	0.13	0.14
	assign (segid 3A4 and resid 219 and name CB)	(segid 3A4 and resid 223 and name CA)	7.37	0.13	0.13
	assign (segid 3A4 and resid 219 and name CB)	(segid 3A4 and resid 223 and name CB)	7.19	0.19	0.19
5	assign (segid 3A4 and resid 219 and name CB)	(segid 3A4 and resid 223 and name N)	6.24	0.12	0.12
	assign (segid 3A4 and resid 219 and name CB)	(segid 3A4 and resid 224 and name CA)	9.42	0.08	0.08
	assign (segid 3A4 and resid 219 and name CB)	(segid 3A4 and resid 224 and name CB)	9.32	0.09	0.09
	assign (segid 3A4 and resid 219 and name CB)	(segid 3A4 and resid 225 and name CA)	10.41	0.12	0.13
	assign (segid 3A4 and resid 219 and name CB)	(segid 3A4 and resid 225 and name CB)	9.78	0.12	0.13
10	assign (segid 3A4 and resid 219 and name CB)	(segid 3A4 and resid 226 and name CA)	11.73	0.22	0.22
	assign (segid 3A4 and resid 219 and name CB)	(segid 3A4 and resid 240 and name CA)	17.97	0.58	0.57
	assign (segid 3A4 and resid 219 and name CB)	(segid 3A4 and resid 241 and name CA)	16.28	0.65	0.65
	assign (segid 3A4 and resid 219 and name CB)	(segid 3A4 and resid 241 and name CB)	16.88	0.72	0.72
	assign (segid 3A4 and resid 219 and name CB)	(segid 3A4 and resid 242 and name CA)	17.98	0.64	0.64
15	assign (segid 3A4 and resid 219 and name CB)	(segid 3A4 and resid 243 and name CA)	16.87	0.39	0.39
	assign (segid 3A4 and resid 219 and name CB)	(segid 3A4 and resid 243 and name CB)	17.27	0.35	0.35
	assign (segid 3A4 and resid 219 and name CB)	(segid 3A4 and resid 244 and name CA)	13.18	0.45	0.44
	assign (segid 3A4 and resid 219 and name CB)	(segid 3A4 and resid 244 and name CB)	12.66	0.51	0.50
	assign (segid 3A4 and resid 219 and name CB)	(segid 3A4 and resid 245 and name CA)	13.89	0.46	0.46
20	assign (segid 3A4 and resid 219 and name CB)	(segid 3A4 and resid 245 and name CB)	15.02	0.46	0.45
	assign (segid 3A4 and resid 219 and name CB)	(segid 3A4 and resid 246 and name CA)	15.99	0.38	0.38
	assign (segid 3A4 and resid 219 and name CB)	(segid 3A4 and resid 246 and name CB)	17.25	0.41	0.41
	assign (segid 3A4 and resid 219 and name CB)	(segid 3A4 and resid 247 and name CA)	13.60	0.37	0.36
	assign (segid 3A4 and resid 219 and name CB)	(segid 3A4 and resid 247 and name CB)	13.03	0.41	0.41
25	assign (segid 3A4 and resid 219 and name CB)	(segid 3A4 and resid 248 and name CA)	10.98	0.30	0.31
	assign (segid 3A4 and resid 219 and name CB)	(segid 3A4 and resid 248 and name CB)	10.43	0.36	0.35
	assign (segid 3A4 and resid 219 and name CB)	(segid 3A4 and resid 249 and name CA)	14.13	0.34	0.35
	assign (segid 3A4 and resid 219 and name CB)	(segid 3A4 and resid 250 and name CA)	15.36	0.28	0.28
	assign (segid 3A4 and resid 219 and name CB)	(segid 3A4 and resid 250 and name CB)	15.82	0.35	0.35
30	assign (segid 3A4 and resid 219 and name CB)	(segid 3A4 and resid 251 and name CA)	12.49	0.21	0.22
	assign (segid 3A4 and resid 219 and name CB)	(segid 3A4 and resid 251 and name CB)	11.10	0.19	0.19
	assign (segid 3A4 and resid 219 and name CB)	(segid 3A4 and resid 252 and name CA)	12.86	0.42	0.43
	assign (segid 3A4 and resid 219 and name CB)	(segid 3A4 and resid 252 and name CB)	12.80	0.45	0.44
	assign (segid 3A4 and resid 219 and name CB)	(segid 3A4 and resid 253 and name CA)	16.61	0.40	0.40
35	assign (segid 3A4 and resid 219 and name CB)	(segid 3A4 and resid 254 and name CA)	17.19	0.49	0.49
	assign (segid 3A4 and resid 219 and name CB)	(segid 3A4 and resid 255 and name CA)	15.35	1.21	1.21
	assign (segid 3A4 and resid 219 and name CB)	(segid 3A4 and resid 256 and name CA)	16.55	0.48	0.48
	assign (segid 3A4 and resid 219 and name CB)	(segid 3A4 and resid 259 and name CB)	18.39	0.51	0.51
	assign (segid 3A4 and resid 219 and name CB)	(segid 3A4 and resid 392 and name CA)	17.00	0.58	0.58
40	assign (segid 3A4 and resid 219 and name CB)	(segid 3A4 and resid 392 and name CB)	16.17	0.48	0.49
	assign (segid 3A4 and resid 219 and name CB)	(segid 3A4 and resid 393 and name CA)	15.52	0.61	0.62
	assign (segid 3A4 and resid 219 and name CB)	(segid 3A4 and resid 394 and name CA)	18.77	0.68	0.68
	assign (segid 3A4 and resid 219 and name CB)	(segid 3A4 and resid 395 and name CA)	17.58	0.87	0.88
	assign (segid 3A4 and resid 219 and name CB)	(segid 3A4 and resid 396 and name CA)	14.87	0.90	0.90
45	assign (segid 3A4 and resid 219 and name CB)	(segid 3A4 and resid 396 and name CB)	13.58	0.87	0.87
	assign (segid 3A4 and resid 219 and name CB)	(segid 3A4 and resid 397 and name CA)	17.56	0.88	0.87
	assign (segid 3A4 and resid 219 and name CB)	(segid 3A4 and resid 397 and name CB)	18.32	0.83	0.82
	assign (segid 3A4 and resid 219 and name CB)	(segid 3A4 and resid 399 and name CB)	17.11	1.03	1.02
50	assign (segid 3A4 and resid 219 and name CB)	(segid 3A4 and resid 400 and name CA)	17.64	1.11	1.10
	assign (segid 3A4 and resid 219 and name CB)	(segid 3A4 and resid 400 and name CB)	16.84	1.10	1.11
	assign (segid 3A4 and resid 219 and name CG)	(segid 3A4 and resid 220 and name C)	4.80	0.13	0.12
	assign (segid 3A4 and resid 219 and name CG)	(segid 3A4 and resid 220 and name CA)	4.87	0.10	0.10
	assign (segid 3A4 and resid 219 and name CG)	(segid 3A4 and resid 220 and name CB)	5.87	0.20	0.19
	assign (segid 3A4 and resid 219 and name CG)	(segid 3A4 and resid 220 and name N)	3.79	0.09	0.08
55	assign (segid 3A4 and resid 219 and name CG)	(segid 3A4 and resid 220 and name O)	5.73	0.14	0.15
	assign (segid 3A4 and resid 219 and name CG)	(segid 3A4 and resid 221 and name C)	4.83	0.21	0.21
	assign (segid 3A4 and resid 219 and name CG)	(segid 3A4 and resid 221 and name CA)	4.72	0.17	0.17
	assign (segid 3A4 and resid 219 and name CG)	(segid 3A4 and resid 221 and name CB)	4.58	0.16	0.15
	assign (segid 3A4 and resid 219 and name CG)	(segid 3A4 and resid 221 and name N)	4.13	0.13	0.13
60	assign (segid 3A4 and resid 219 and name CG)	(segid 3A4 and resid 221 and name O)	6.01	0.21	0.21
	assign (segid 3A4 and resid 219 and name CG)	(segid 3A4 and resid 222 and name C)	5.81	0.21	0.21
	assign (segid 3A4 and resid 219 and name CG)	(segid 3A4 and resid 222 and name CA)	4.70	0.23	0.23
	assign (segid 3A4 and resid 219 and name CG)	(segid 3A4 and resid 222 and name CB)	4.18	0.28	0.28
	assign (segid 3A4 and resid 219 and name CG)	(segid 3A4 and resid 222 and name N)	3.96	0.21	0.21
65	assign (segid 3A4 and resid 219 and name CG)	(segid 3A4 and resid 222 and name O)	6.95	0.22	0.21
	assign (segid 3A4 and resid 219 and name CG)	(segid 3A4 and resid 223 and name CA)	7.05	0.18	0.19
	assign (segid 3A4 and resid 219 and name CG)	(segid 3A4 and resid 223 and name CB)	7.19	0.20	0.19
	assign (segid 3A4 and resid 219 and name CG)	(segid 3A4 and resid 223 and name N)	5.75	0.20	0.20
	assign (segid 3A4 and resid 219 and name N)	(segid 3A4 and resid 219 and name C)	2.45	0.05	0.04
70	assign (segid 3A4 and resid 219 and name N)	(segid 3A4 and resid 219 and name CA)	1.45	0.01	0.01
	assign (segid 3A4 and resid 219 and name N)	(segid 3A4 and resid 219 and name CB)	2.44	0.03	0.02
	assign (segid 3A4 and resid 219 and name N)	(segid 3A4 and resid 219 and name CG)	3.00	0.04	0.04
	assign (segid 3A4 and resid 219 and name N)	(segid 3A4 and resid 219 and name O)	2.70	0.07	0.06
	assign (segid 3A4 and resid 219 and name N)	(segid 3A4 and resid 220 and name C)	5.36	0.08	0.08
75	assign (segid 3A4 and resid 219 and name N)	(segid 3A4 and resid 220 and name CA)	4.86	0.07	0.07
	assign (segid 3A4 and resid 219 and name N)	(segid 3A4 and resid 220 and name CB)	6.07	0.05	0.06
	assign (segid 3A4 and resid 219 and name N)	(segid 3A4 and resid 220 and name N)	3.65	0.04	0.03
	assign (segid 3A4 and resid 219 and name N)	(segid 3A4 and resid 220 and name O)	6.06	0.14	0.14
	assign (segid 3A4 and resid 219 and name N)	(segid 3A4 and resid 221 and name C)	6.16	0.08	0.08
80	assign (segid 3A4 and resid 219 and name N)	(segid 3A4 and resid 221 and name CA)	6.36	0.06	0.06
	assign (segid 3A4 and resid 219 and name N)	(segid 3A4 and resid 221 and name CB)	6.82	0.10	0.11
	assign (segid 3A4 and resid 219 and name N)	(segid 3A4 and resid 221 and name N)	5.43	0.07	0.06
	assign (segid 3A4 and resid 219 and name N)	(segid 3A4 and resid 221 and name O)	7.20	0.12	0.11

	assign (segid 3A4 and resid 219 and name N)	(segid 3A4 and resid 222 and name C)	5.88	0.20	0.20
	assign (segid 3A4 and resid 219 and name N)	(segid 3A4 and resid 222 and name CA)	5.37	0.16	0.15
	assign (segid 3A4 and resid 219 and name N)	(segid 3A4 and resid 222 and name CB)	4.45	0.25	0.25
	assign (segid 3A4 and resid 219 and name N)	(segid 3A4 and resid 222 and name N)	5.10	0.07	0.07
	assign (segid 3A4 and resid 219 and name N)	(segid 3A4 and resid 222 and name O)	6.98	0.23	0.22
5	assign (segid 3A4 and resid 219 and name N)	(segid 3A4 and resid 223 and name CA)	6.34	0.25	0.24
	assign (segid 3A4 and resid 219 and name N)	(segid 3A4 and resid 223 and name CB)	6.09	0.28	0.27
	assign (segid 3A4 and resid 219 and name N)	(segid 3A4 and resid 223 and name N)	5.41	0.21	0.21
	assign (segid 3A4 and resid 219 and name N)	(segid 3A4 and resid 219 and name CB)	3.39	0.04	0.05
	assign (segid 3A4 and resid 219 and name O)	(segid 3A4 and resid 219 and name CG)	3.52	0.14	0.13
10	assign (segid 3A4 and resid 219 and name O)	(segid 3A4 and resid 220 and name C)	2.94	0.10	0.10
	assign (segid 3A4 and resid 219 and name O)	(segid 3A4 and resid 220 and name CA)	2.75	0.05	0.05
	assign (segid 3A4 and resid 219 and name O)	(segid 3A4 and resid 220 and name CB)	4.23	0.05	0.04
	assign (segid 3A4 and resid 219 and name O)	(segid 3A4 and resid 220 and name N)	2.24	0.02	0.01
	assign (segid 3A4 and resid 219 and name O)	(segid 3A4 and resid 220 and name O)	3.44	0.16	0.15
15	assign (segid 3A4 and resid 219 and name O)	(segid 3A4 and resid 221 and name C)	4.09	0.20	0.21
	assign (segid 3A4 and resid 219 and name O)	(segid 3A4 and resid 221 and name CA)	4.32	0.16	0.17
	assign (segid 3A4 and resid 219 and name O)	(segid 3A4 and resid 221 and name CB)	5.26	0.21	0.21
	assign (segid 3A4 and resid 219 and name O)	(segid 3A4 and resid 221 and name N)	3.36	0.10	0.11
	assign (segid 3A4 and resid 219 and name O)	(segid 3A4 and resid 221 and name O)	5.02	0.24	0.24
20	assign (segid 3A4 and resid 219 and name O)	(segid 3A4 and resid 222 and name C)	4.01	0.17	0.17
	assign (segid 3A4 and resid 219 and name O)	(segid 3A4 and resid 222 and name CA)	3.86	0.20	0.20
	assign (segid 3A4 and resid 219 and name O)	(segid 3A4 and resid 222 and name CB)	3.71	0.25	0.25
	assign (segid 3A4 and resid 219 and name O)	(segid 3A4 and resid 222 and name N)	3.32	0.16	0.17
	assign (segid 3A4 and resid 219 and name O)	(segid 3A4 and resid 222 and name O)	5.21	0.17	0.16
25	assign (segid 3A4 and resid 219 and name O)	(segid 3A4 and resid 223 and name C)	5.26	0.14	0.13
	assign (segid 3A4 and resid 219 and name O)	(segid 3A4 and resid 223 and name CA)	4.12	0.16	0.15
	assign (segid 3A4 and resid 219 and name O)	(segid 3A4 and resid 223 and name CB)	3.84	0.18	0.19
	assign (segid 3A4 and resid 219 and name O)	(segid 3A4 and resid 223 and name N)	3.22	0.15	0.15
	assign (segid 3A4 and resid 219 and name O)	(segid 3A4 and resid 223 and name O)	6.38	0.13	0.14
30	assign (segid 3A4 and resid 219 and name O)	(segid 3A4 and resid 224 and name C)	7.44	0.18	0.18
	assign (segid 3A4 and resid 219 and name O)	(segid 3A4 and resid 224 and name CA)	6.63	0.15	0.15
	assign (segid 3A4 and resid 219 and name O)	(segid 3A4 and resid 224 and name CB)	6.86	0.17	0.17
	assign (segid 3A4 and resid 219 and name O)	(segid 3A4 and resid 224 and name N)	5.27	0.15	0.15
	assign (segid 3A4 and resid 219 and name O)	(segid 3A4 and resid 225 and name N)	7.08	0.18	0.19
35	assign (segid 3A4 and resid 21 and name O)	(segid 3A4 and resid 21 and name CB)	2.50	0.04	0.04
	assign (segid 3A4 and resid 21 and name C)	(segid 3A4 and resid 21 and name O)	1.23	0.01	0.00
	assign (segid 3A4 and resid 21 and name C)	(segid 3A4 and resid 22 and name C)	3.28	0.12	0.12
	assign (segid 3A4 and resid 21 and name C)	(segid 3A4 and resid 22 and name CA)	2.42	0.01	0.01
	assign (segid 3A4 and resid 21 and name C)	(segid 3A4 and resid 22 and name N)	1.32	0.01	0.02
40	assign (segid 3A4 and resid 21 and name C)	(segid 3A4 and resid 22 and name O)	3.66	0.19	0.19
	assign (segid 3A4 and resid 21 and name C)	(segid 3A4 and resid 23 and name C)	6.53	0.13	0.13
	assign (segid 3A4 and resid 21 and name C)	(segid 3A4 and resid 23 and name CA)	5.38	0.16	0.16
	assign (segid 3A4 and resid 21 and name C)	(segid 3A4 and resid 23 and name CB)	5.79	0.24	0.24
	assign (segid 3A4 and resid 21 and name C)	(segid 3A4 and resid 23 and name N)	4.16	0.14	0.14
45	assign (segid 3A4 and resid 21 and name C)	(segid 3A4 and resid 23 and name O)	6.62	0.07	0.08
	assign (segid 3A4 and resid 21 and name C)	(segid 3A4 and resid 30 and name C)	5.44	0.12	0.13
	assign (segid 3A4 and resid 21 and name C)	(segid 3A4 and resid 30 and name CA)	6.89	0.13	0.13
	assign (segid 3A4 and resid 21 and name C)	(segid 3A4 and resid 30 and name N)	7.14	0.13	0.14
	assign (segid 3A4 and resid 21 and name C)	(segid 3A4 and resid 30 and name O)	4.67	0.18	0.19
50	assign (segid 3A4 and resid 21 and name C)	(segid 3A4 and resid 31 and name C)	4.63	0.05	0.06
	assign (segid 3A4 and resid 21 and name C)	(segid 3A4 and resid 31 and name CA)	4.25	0.07	0.08
	assign (segid 3A4 and resid 21 and name C)	(segid 3A4 and resid 31 and name CB)	4.78	0.16	0.16
	assign (segid 3A4 and resid 21 and name C)	(segid 3A4 and resid 31 and name N)	5.33	0.09	0.08
	assign (segid 3A4 and resid 21 and name C)	(segid 3A4 and resid 31 and name O)	5.84	0.06	0.06
55	assign (segid 3A4 and resid 21 and name C)	(segid 3A4 and resid 32 and name C)	5.19	0.25	0.25
	assign (segid 3A4 and resid 21 and name C)	(segid 3A4 and resid 32 and name CA)	4.97	0.21	0.20
	assign (segid 3A4 and resid 21 and name C)	(segid 3A4 and resid 32 and name CB)	5.01	0.25	0.25
	assign (segid 3A4 and resid 21 and name C)	(segid 3A4 and resid 32 and name N)	3.99	0.13	0.13
	assign (segid 3A4 and resid 21 and name C)	(segid 3A4 and resid 32 and name O)	4.49	0.34	0.34
60	assign (segid 3A4 and resid 21 and name C)	(segid 3A4 and resid 33 and name CA)	7.16	0.24	0.24
	assign (segid 3A4 and resid 21 and name C)	(segid 3A4 and resid 33 and name N)	6.42	0.21	0.21
	assign (segid 3A4 and resid 21 and name CA)	(segid 3A4 and resid 21 and name CB)	1.52	0.01	0.01
	assign (segid 3A4 and resid 21 and name CA)	(segid 3A4 and resid 21 and name O)	1.53	0.01	0.02
65	assign (segid 3A4 and resid 21 and name CA)	(segid 3A4 and resid 22 and name C)	2.37	0.01	0.01
	assign (segid 3A4 and resid 21 and name CA)	(segid 3A4 and resid 22 and name CA)	4.52	0.10	0.10
	assign (segid 3A4 and resid 21 and name CA)	(segid 3A4 and resid 22 and name N)	3.77	0.01	0.02
	assign (segid 3A4 and resid 21 and name CA)	(segid 3A4 and resid 22 and name O)	2.40	0.02	0.03
	assign (segid 3A4 and resid 21 and name CA)	(segid 3A4 and resid 22 and name O)	4.59	0.16	0.15
70	assign (segid 3A4 and resid 21 and name CA)	(segid 3A4 and resid 23 and name CB)	6.61	0.14	0.14
	assign (segid 3A4 and resid 21 and name CA)	(segid 3A4 and resid 23 and name N)	6.95	0.22	0.21
	assign (segid 3A4 and resid 21 and name CA)	(segid 3A4 and resid 23 and name O)	5.51	0.13	0.13
	assign (segid 3A4 and resid 21 and name CA)	(segid 3A4 and resid 24 and name CA)	10.16	0.19	0.18
	assign (segid 3A4 and resid 21 and name CA)	(segid 3A4 and resid 24 and name CB)	10.71	0.37	0.38
	assign (segid 3A4 and resid 21 and name CA)	(segid 3A4 and resid 25 and name CA)	12.81	0.38	0.37
75	assign (segid 3A4 and resid 21 and name CA)	(segid 3A4 and resid 26 and name CA)	16.01	0.82	0.82
	assign (segid 3A4 and resid 21 and name CA)	(segid 3A4 and resid 29 and name CA)	10.23	0.19	0.19
	assign (segid 3A4 and resid 21 and name CA)	(segid 3A4 and resid 30 and name C)	6.88	0.14	0.15
	assign (segid 3A4 and resid 21 and name CA)	(segid 3A4 and resid 30 and name CA)	8.36	0.15	0.15
80	assign (segid 3A4 and resid 21 and name CA)	(segid 3A4 and resid 30 and name O)	6.16	0.19	0.19
	assign (segid 3A4 and resid 21 and name CA)	(segid 3A4 and resid 31 and name C)	5.65	0.06	0.06
	assign (segid 3A4 and resid 21 and name CA)	(segid 3A4 and resid 31 and name CA)	5.45	0.10	0.09
	assign (segid 3A4 and resid 21 and name CA)	(segid 3A4 and resid 31 and name CB)	5.75	0.15	0.14

	assign (segid 3A4 and resid 21 and name CA) (segid 3A4 and resid 31 and name N)	6.65	0.11	0.11
	assign (segid 3A4 and resid 21 and name CA) (segid 3A4 and resid 31 and name O)	6.82	0.07	0.07
	assign (segid 3A4 and resid 21 and name CA) (segid 3A4 and resid 322 and name CA)	14.54	0.44	0.44
	assign (segid 3A4 and resid 21 and name CA) (segid 3A4 and resid 323 and name CA)	14.80	0.11	0.12
	assign (segid 3A4 and resid 21 and name CA) (segid 3A4 and resid 323 and name CB)	14.48	0.24	0.23
5	assign (segid 3A4 and resid 21 and name CA) (segid 3A4 and resid 324 and name CA)	15.12	0.15	0.14
	assign (segid 3A4 and resid 21 and name CA) (segid 3A4 and resid 324 and name CB)	16.26	0.20	0.21
	assign (segid 3A4 and resid 21 and name CA) (segid 3A4 and resid 325 and name CA)	15.09	0.38	0.38
	assign (segid 3A4 and resid 21 and name CA) (segid 3A4 and resid 325 and name CB)	14.11	0.50	0.50
	assign (segid 3A4 and resid 21 and name CA) (segid 3A4 and resid 326 and name CA)	18.75	0.46	0.46
10	assign (segid 3A4 and resid 21 and name CA) (segid 3A4 and resid 328 and name CA)	16.32	0.90	0.90
	assign (segid 3A4 and resid 21 and name CA) (segid 3A4 and resid 328 and name CB)	16.88	0.98	0.97
	assign (segid 3A4 and resid 21 and name CA) (segid 3A4 and resid 329 and name CA)	14.77	0.91	0.91
	assign (segid 3A4 and resid 21 and name CA) (segid 3A4 and resid 329 and name CB)	14.64	0.94	0.94
	assign (segid 3A4 and resid 21 and name CA) (segid 3A4 and resid 32 and name C)	5.37	0.26	0.26
15	assign (segid 3A4 and resid 21 and name CA) (segid 3A4 and resid 32 and name CA)	5.54	0.19	0.19
	assign (segid 3A4 and resid 21 and name CA) (segid 3A4 and resid 32 and name CB)	5.55	0.24	0.23
	assign (segid 3A4 and resid 21 and name CA) (segid 3A4 and resid 32 and name N)	4.82	0.09	0.09
	assign (segid 3A4 and resid 21 and name CA) (segid 3A4 and resid 32 and name O)	4.41	0.37	0.36
	assign (segid 3A4 and resid 21 and name CA) (segid 3A4 and resid 330 and name CA)	13.18	0.83	0.83
20	assign (segid 3A4 and resid 21 and name CA) (segid 3A4 and resid 330 and name CB)	14.12	0.84	0.84
	assign (segid 3A4 and resid 21 and name CA) (segid 3A4 and resid 331 and name CA)	11.17	0.73	0.73
	assign (segid 3A4 and resid 21 and name CA) (segid 3A4 and resid 331 and name CB)	10.32	0.60	0.60
	assign (segid 3A4 and resid 21 and name CA) (segid 3A4 and resid 332 and name CA)	11.22	1.06	1.06
	assign (segid 3A4 and resid 21 and name CA) (segid 3A4 and resid 333 and name CA)	11.87	1.54	1.53
25	assign (segid 3A4 and resid 21 and name CA) (segid 3A4 and resid 335 and name CA)	8.98	0.82	0.81
	assign (segid 3A4 and resid 21 and name CA) (segid 3A4 and resid 336 and name CA)	11.13	0.73	0.73
	assign (segid 3A4 and resid 21 and name CA) (segid 3A4 and resid 336 and name CB)	12.14	0.68	0.67
	assign (segid 3A4 and resid 21 and name CA) (segid 3A4 and resid 337 and name CA)	10.73	0.90	0.89
	assign (segid 3A4 and resid 21 and name CA) (segid 3A4 and resid 337 and name CB)	10.49	0.84	0.84
30	assign (segid 3A4 and resid 21 and name CA) (segid 3A4 and resid 338 and name CA)	13.63	0.90	0.91
	assign (segid 3A4 and resid 21 and name CA) (segid 3A4 and resid 338 and name CB)	13.79	0.98	0.99
	assign (segid 3A4 and resid 21 and name CA) (segid 3A4 and resid 339 and name CA)	16.35	0.73	0.73
	assign (segid 3A4 and resid 21 and name CA) (segid 3A4 and resid 339 and name CB)	17.81	0.75	0.76
35	assign (segid 3A4 and resid 21 and name CA) (segid 3A4 and resid 33 and name CA)	7.01	0.30	0.30
	assign (segid 3A4 and resid 21 and name CA) (segid 3A4 and resid 33 and name CB)	8.13	0.32	0.32
	assign (segid 3A4 and resid 21 and name CA) (segid 3A4 and resid 33 and name N)	6.54	0.25	0.25
	assign (segid 3A4 and resid 21 and name CA) (segid 3A4 and resid 340 and name CA)	16.15	0.36	0.36
	assign (segid 3A4 and resid 21 and name CA) (segid 3A4 and resid 341 and name CA)	12.44	0.34	0.33
40	assign (segid 3A4 and resid 21 and name CA) (segid 3A4 and resid 341 and name CB)	11.36	0.40	0.40
	assign (segid 3A4 and resid 21 and name CA) (segid 3A4 and resid 342 and name CA)	11.78	0.15	0.16
	assign (segid 3A4 and resid 21 and name CA) (segid 3A4 and resid 343 and name CA)	9.78	0.22	0.22
	assign (segid 3A4 and resid 21 and name CA) (segid 3A4 and resid 343 and name CB)	10.01	0.35	0.35
	assign (segid 3A4 and resid 21 and name CA) (segid 3A4 and resid 344 and name CA)	10.20	0.21	0.21
	assign (segid 3A4 and resid 21 and name CA) (segid 3A4 and resid 344 and name CB)	9.94	0.32	0.32
45	assign (segid 3A4 and resid 21 and name CA) (segid 3A4 and resid 345 and name CA)	11.21	0.36	0.36
	assign (segid 3A4 and resid 21 and name CA) (segid 3A4 and resid 345 and name CB)	12.29	0.42	0.41
	assign (segid 3A4 and resid 21 and name CA) (segid 3A4 and resid 346 and name CA)	11.91	0.49	0.49
	assign (segid 3A4 and resid 21 and name CA) (segid 3A4 and resid 346 and name CB)	11.02	0.54	0.55
50	assign (segid 3A4 and resid 21 and name CA) (segid 3A4 and resid 347 and name CA)	15.33	0.48	0.47
	assign (segid 3A4 and resid 21 and name CA) (segid 3A4 and resid 347 and name CB)	16.56	0.49	0.48
	assign (segid 3A4 and resid 21 and name CA) (segid 3A4 and resid 348 and name CA)	16.11	0.39	0.40
	assign (segid 3A4 and resid 21 and name CA) (segid 3A4 and resid 349 and name CA)	13.52	0.43	0.44
	assign (segid 3A4 and resid 21 and name CA) (segid 3A4 and resid 349 and name CB)	12.03	0.43	0.43
55	assign (segid 3A4 and resid 21 and name CA) (segid 3A4 and resid 34 and name CA)	8.58	0.38	0.39
	assign (segid 3A4 and resid 21 and name CA) (segid 3A4 and resid 34 and name CB)	8.03	0.43	0.43
	assign (segid 3A4 and resid 21 and name CA) (segid 3A4 and resid 350 and name CA)	14.85	0.76	0.76
	assign (segid 3A4 and resid 21 and name CA) (segid 3A4 and resid 350 and name CB)	15.10	0.85	0.85
	assign (segid 3A4 and resid 21 and name CA) (segid 3A4 and resid 351 and name CA)	18.27	0.63	0.64
60	assign (segid 3A4 and resid 21 and name CA) (segid 3A4 and resid 352 and name CA)	17.66	0.75	0.75
	assign (segid 3A4 and resid 21 and name CA) (segid 3A4 and resid 352 and name CB)	17.29	0.83	0.82
	assign (segid 3A4 and resid 21 and name CA) (segid 3A4 and resid 353 and name CA)	16.28	0.84	0.84
	assign (segid 3A4 and resid 21 and name CA) (segid 3A4 and resid 353 and name CB)	15.82	0.94	0.95
	assign (segid 3A4 and resid 21 and name CA) (segid 3A4 and resid 35 and name CA)	10.97	0.35	0.35
65	assign (segid 3A4 and resid 21 and name CA) (segid 3A4 and resid 36 and name CA)	14.32	0.30	0.31
	assign (segid 3A4 and resid 21 and name CA) (segid 3A4 and resid 37 and name CA)	14.49	0.22	0.22
	assign (segid 3A4 and resid 21 and name CA) (segid 3A4 and resid 37 and name CB)	14.49	0.27	0.27
	assign (segid 3A4 and resid 21 and name CA) (segid 3A4 and resid 382 and name CA)	18.61	0.43	0.43
	assign (segid 3A4 and resid 21 and name CA) (segid 3A4 and resid 38 and name CA)	11.51	0.35	0.35
70	assign (segid 3A4 and resid 21 and name CA) (segid 3A4 and resid 38 and name CB)	10.06	0.32	0.33
	assign (segid 3A4 and resid 21 and name CA) (segid 3A4 and resid 39 and name CA)	12.77	0.36	0.35
	assign (segid 3A4 and resid 21 and name CA) (segid 3A4 and resid 39 and name CB)	13.03	0.39	0.39
	assign (segid 3A4 and resid 21 and name CA) (segid 3A4 and resid 40 and name CA)	16.25	0.31	0.32
	assign (segid 3A4 and resid 21 and name CA) (segid 3A4 and resid 40 and name CB)	17.11	0.29	0.29
75	assign (segid 3A4 and resid 21 and name CA) (segid 3A4 and resid 41 and name CA)	15.45	0.29	0.28
	assign (segid 3A4 and resid 21 and name CA) (segid 3A4 and resid 41 and name CB)	14.62	0.30	0.29
	assign (segid 3A4 and resid 21 and name CA) (segid 3A4 and resid 42 and name CA)	13.90	0.32	0.33
	assign (segid 3A4 and resid 21 and name CA) (segid 3A4 and resid 42 and name CB)	12.63	0.33	0.33
	assign (segid 3A4 and resid 21 and name CB) (segid 3A4 and resid 22 and name C)	4.69	0.07	0.07
80	assign (segid 3A4 and resid 21 and name CB) (segid 3A4 and resid 22 and name CA)	4.41	0.08	0.07
	assign (segid 3A4 and resid 21 and name CB) (segid 3A4 and resid 22 and name N)	3.10	0.09	0.09
	assign (segid 3A4 and resid 21 and name CB) (segid 3A4 and resid 22 and name O)	4.42	0.12	0.12
	assign (segid 3A4 and resid 21 and name CB) (segid 3A4 and resid 23 and name CA)	6.52	0.14	0.15

	assign	(segid 3A4 and resid 21 and name CB)	(segid 3A4 and resid 23 and name CB)	6.73	0.22	0.23
	assign	(segid 3A4 and resid 21 and name CB)	(segid 3A4 and resid 23 and name N)	5.68	0.12	0.13
	assign	(segid 3A4 and resid 21 and name CB)	(segid 3A4 and resid 24 and name CA)	10.17	0.19	0.18
	assign	(segid 3A4 and resid 21 and name CB)	(segid 3A4 and resid 24 and name CB)	10.69	0.31	0.30
5	assign	(segid 3A4 and resid 21 and name CB)	(segid 3A4 and resid 25 and name CA)	12.73	0.48	0.48
	assign	(segid 3A4 and resid 21 and name CB)	(segid 3A4 and resid 26 and name CA)	16.01	0.86	0.86
	assign	(segid 3A4 and resid 21 and name CB)	(segid 3A4 and resid 29 and name CA)	10.85	0.19	0.18
	assign	(segid 3A4 and resid 21 and name CB)	(segid 3A4 and resid 30 and name C)	7.73	0.10	0.09
	assign	(segid 3A4 and resid 21 and name CB)	(segid 3A4 and resid 30 and name CA)	9.16	0.11	0.10
10	assign	(segid 3A4 and resid 21 and name CB)	(segid 3A4 and resid 30 and name O)	6.86	0.13	0.13
	assign	(segid 3A4 and resid 21 and name CB)	(segid 3A4 and resid 31 and name C)	6.57	0.12	0.12
	assign	(segid 3A4 and resid 21 and name CB)	(segid 3A4 and resid 31 and name CA)	6.55	0.08	0.07
	assign	(segid 3A4 and resid 21 and name CB)	(segid 3A4 and resid 31 and name CB)	7.05	0.12	0.13
	assign	(segid 3A4 and resid 21 and name CB)	(segid 3A4 and resid 31 and name N)	7.66	0.07	0.07
15	assign	(segid 3A4 and resid 21 and name CB)	(segid 3A4 and resid 31 and name O)	7.70	0.15	0.15
	assign	(segid 3A4 and resid 21 and name CB)	(segid 3A4 and resid 322 and name CA)	15.28	0.48	0.48
	assign	(segid 3A4 and resid 21 and name CB)	(segid 3A4 and resid 323 and name CA)	15.84	0.11	0.11
	assign	(segid 3A4 and resid 21 and name CB)	(segid 3A4 and resid 323 and name CB)	15.55	0.22	0.22
	assign	(segid 3A4 and resid 21 and name CB)	(segid 3A4 and resid 324 and name CA)	16.33	0.14	0.15
20	assign	(segid 3A4 and resid 21 and name CB)	(segid 3A4 and resid 324 and name CB)	17.46	0.24	0.23
	assign	(segid 3A4 and resid 21 and name CB)	(segid 3A4 and resid 325 and name CA)	16.48	0.36	0.36
	assign	(segid 3A4 and resid 21 and name CB)	(segid 3A4 and resid 325 and name CB)	15.54	0.48	0.49
	assign	(segid 3A4 and resid 21 and name CB)	(segid 3A4 and resid 328 and name CA)	17.82	0.93	0.92
	assign	(segid 3A4 and resid 21 and name CB)	(segid 3A4 and resid 329 and name CA)	16.26	0.95	0.94
25	assign	(segid 3A4 and resid 21 and name CB)	(segid 3A4 and resid 329 and name CB)	16.12	0.95	0.96
	assign	(segid 3A4 and resid 21 and name CB)	(segid 3A4 and resid 32 and name C)	5.93	0.35	0.36
	assign	(segid 3A4 and resid 21 and name CB)	(segid 3A4 and resid 32 and name CA)	6.06	0.29	0.29
	assign	(segid 3A4 and resid 21 and name CB)	(segid 3A4 and resid 32 and name CB)	5.68	0.35	0.35
	assign	(segid 3A4 and resid 21 and name CB)	(segid 3A4 and resid 32 and name N)	5.59	0.16	0.17
30	assign	(segid 3A4 and resid 21 and name CB)	(segid 3A4 and resid 32 and name O)	4.96	0.44	0.43
	assign	(segid 3A4 and resid 21 and name CB)	(segid 3A4 and resid 330 and name CA)	14.58	0.89	0.90
	assign	(segid 3A4 and resid 21 and name CB)	(segid 3A4 and resid 330 and name CB)	15.48	0.92	0.93
	assign	(segid 3A4 and resid 21 and name CB)	(segid 3A4 and resid 331 and name CA)	12.47	0.79	0.79
	assign	(segid 3A4 and resid 21 and name CB)	(segid 3A4 and resid 331 and name CB)	11.65	0.66	0.65
35	assign	(segid 3A4 and resid 21 and name CB)	(segid 3A4 and resid 332 and name CA)	12.23	1.19	1.18
	assign	(segid 3A4 and resid 21 and name CB)	(segid 3A4 and resid 333 and name CA)	12.89	1.67	1.66
	assign	(segid 3A4 and resid 21 and name CB)	(segid 3A4 and resid 335 and name CA)	10.23	0.92	0.93
	assign	(segid 3A4 and resid 21 and name CB)	(segid 3A4 and resid 336 and name CA)	12.54	0.81	0.81
	assign	(segid 3A4 and resid 21 and name CB)	(segid 3A4 and resid 336 and name CB)	13.50	0.78	0.78
40	assign	(segid 3A4 and resid 21 and name CB)	(segid 3A4 and resid 337 and name CA)	12.23	0.92	0.91
	assign	(segid 3A4 and resid 21 and name CB)	(segid 3A4 and resid 337 and name CB)	12.00	0.85	0.85
	assign	(segid 3A4 and resid 21 and name CB)	(segid 3A4 and resid 338 and name CA)	15.07	0.92	0.92
	assign	(segid 3A4 and resid 21 and name CB)	(segid 3A4 and resid 338 and name CB)	15.18	1.00	1.01
	assign	(segid 3A4 and resid 21 and name CB)	(segid 3A4 and resid 339 and name CA)	17.78	0.72	0.72
45	assign	(segid 3A4 and resid 21 and name CB)	(segid 3A4 and resid 33 and name CA)	7.59	0.40	0.41
	assign	(segid 3A4 and resid 21 and name CB)	(segid 3A4 and resid 33 and name CB)	8.87	0.40	0.40
	assign	(segid 3A4 and resid 21 and name CB)	(segid 3A4 and resid 340 and name CA)	17.46	0.34	0.34
	assign	(segid 3A4 and resid 21 and name CB)	(segid 3A4 and resid 341 and name CA)	13.72	0.32	0.31
	assign	(segid 3A4 and resid 21 and name CB)	(segid 3A4 and resid 341 and name CB)	12.70	0.40	0.39
50	assign	(segid 3A4 and resid 21 and name CB)	(segid 3A4 and resid 342 and name CA)	12.88	0.07	0.06
	assign	(segid 3A4 and resid 21 and name CB)	(segid 3A4 and resid 343 and name CA)	10.85	0.21	0.20
	assign	(segid 3A4 and resid 21 and name CB)	(segid 3A4 and resid 343 and name CB)	11.16	0.32	0.33
	assign	(segid 3A4 and resid 21 and name CB)	(segid 3A4 and resid 344 and name CA)	10.83	0.30	0.30
	assign	(segid 3A4 and resid 21 and name CB)	(segid 3A4 and resid 344 and name CB)	10.41	0.38	0.38
55	assign	(segid 3A4 and resid 21 and name CB)	(segid 3A4 and resid 345 and name CA)	11.74	0.49	0.49
	assign	(segid 3A4 and resid 21 and name CB)	(segid 3A4 and resid 345 and name CB)	12.91	0.52	0.52
	assign	(segid 3A4 and resid 21 and name CB)	(segid 3A4 and resid 346 and name CA)	11.96	0.62	0.63
	assign	(segid 3A4 and resid 21 and name CB)	(segid 3A4 and resid 346 and name CB)	10.93	0.68	0.68
	assign	(segid 3A4 and resid 21 and name CB)	(segid 3A4 and resid 347 and name CA)	15.40	0.61	0.61
60	assign	(segid 3A4 and resid 21 and name CB)	(segid 3A4 and resid 347 and name CB)	16.67	0.62	0.63
	assign	(segid 3A4 and resid 21 and name CB)	(segid 3A4 and resid 348 and name CA)	15.83	0.54	0.54
	assign	(segid 3A4 and resid 21 and name CB)	(segid 3A4 and resid 349 and name CA)	13.15	0.55	0.54
	assign	(segid 3A4 and resid 21 and name CB)	(segid 3A4 and resid 349 and name CB)	11.65	0.55	0.56
	assign	(segid 3A4 and resid 21 and name CB)	(segid 3A4 and resid 34 and name CA)	8.54	0.53	0.52
65	assign	(segid 3A4 and resid 21 and name CB)	(segid 3A4 and resid 34 and name CB)	7.74	0.56	0.57
	assign	(segid 3A4 and resid 21 and name CB)	(segid 3A4 and resid 350 and name CA)	14.77	0.79	0.79
	assign	(segid 3A4 and resid 21 and name CB)	(segid 3A4 and resid 350 and name CB)	15.16	0.86	0.87
	assign	(segid 3A4 and resid 21 and name CB)	(segid 3A4 and resid 351 and name CA)	18.05	0.69	0.70
	assign	(segid 3A4 and resid 21 and name CB)	(segid 3A4 and resid 352 and name CA)	17.16	0.82	0.82
70	assign	(segid 3A4 and resid 21 and name CB)	(segid 3A4 and resid 352 and name CB)	16.70	0.92	0.91
	assign	(segid 3A4 and resid 21 and name CB)	(segid 3A4 and resid 353 and name CA)	15.89	0.86	0.86
	assign	(segid 3A4 and resid 21 and name CB)	(segid 3A4 and resid 353 and name CB)	15.58	0.96	0.95
	assign	(segid 3A4 and resid 21 and name CB)	(segid 3A4 and resid 35 and name CA)	11.06	0.44	0.44
	assign	(segid 3A4 and resid 21 and name CB)	(segid 3A4 and resid 36 and name CA)	14.56	0.43	0.42
75	assign	(segid 3A4 and resid 21 and name CB)	(segid 3A4 and resid 37 and name CA)	14.99	0.26	0.26
	assign	(segid 3A4 and resid 21 and name CB)	(segid 3A4 and resid 37 and name CB)	14.96	0.27	0.27
	assign	(segid 3A4 and resid 21 and name CB)	(segid 3A4 and resid 382 and name CB)	18.90	0.46	0.47
	assign	(segid 3A4 and resid 21 and name CB)	(segid 3A4 and resid 38 and name CA)	12.26	0.42	0.41
	assign	(segid 3A4 and resid 21 and name CB)	(segid 3A4 and resid 38 and name CB)	10.79	0.41	0.40
80	assign	(segid 3A4 and resid 21 and name CB)	(segid 3A4 and resid 39 and name CA)	13.44	0.47	0.46
	assign	(segid 3A4 and resid 21 and name CB)	(segid 3A4 and resid 39 and name CB)	13.55	0.52	0.52
	assign	(segid 3A4 and resid 21 and name CB)	(segid 3A4 and resid 40 and name CA)	16.99	0.40	0.40
	assign	(segid 3A4 and resid 21 and name CB)	(segid 3A4 and resid 40 and name CB)	17.79	0.38	0.38

	assign	(segid 3A4 and resid 21 and name CB)	(segid 3A4 and resid 41 and name CA)	16.44	0.32	0.31
	assign	(segid 3A4 and resid 21 and name CB)	(segid 3A4 and resid 41 and name CB)	15.62	0.33	0.32
	assign	(segid 3A4 and resid 21 and name CB)	(segid 3A4 and resid 42 and name CA)	15.00	0.35	0.36
	assign	(segid 3A4 and resid 21 and name CB)	(segid 3A4 and resid 42 and name CB)	13.70	0.37	0.37
5	assign	(segid 3A4 and resid 21 and name N)	(segid 3A4 and resid 21 and name C)	2.40	0.05	0.05
	assign	(segid 3A4 and resid 21 and name N)	(segid 3A4 and resid 21 and name CA)	1.44	0.01	0.01
	assign	(segid 3A4 and resid 21 and name N)	(segid 3A4 and resid 21 and name CB)	2.44	0.04	0.04
	assign	(segid 3A4 and resid 21 and name N)	(segid 3A4 and resid 21 and name O)	2.63	0.09	0.09
	assign	(segid 3A4 and resid 21 and name N)	(segid 3A4 and resid 22 and name C)	5.62	0.11	0.10
10	assign	(segid 3A4 and resid 21 and name N)	(segid 3A4 and resid 22 and name CA)	4.80	0.05	0.05
	assign	(segid 3A4 and resid 21 and name N)	(segid 3A4 and resid 22 and name N)	3.58	0.06	0.05
	assign	(segid 3A4 and resid 21 and name N)	(segid 3A4 and resid 22 and name O)	5.83	0.16	0.17
	assign	(segid 3A4 and resid 21 and name N)	(segid 3A4 and resid 23 and name CA)	7.56	0.18	0.17
	assign	(segid 3A4 and resid 21 and name N)	(segid 3A4 and resid 23 and name N)	6.44	0.14	0.14
15	assign	(segid 3A4 and resid 21 and name N)	(segid 3A4 and resid 30 and name C)	7.16	0.19	0.18
	assign	(segid 3A4 and resid 21 and name N)	(segid 3A4 and resid 30 and name O)	6.60	0.21	0.22
	assign	(segid 3A4 and resid 21 and name N)	(segid 3A4 and resid 31 and name C)	5.29	0.14	0.14
	assign	(segid 3A4 and resid 21 and name N)	(segid 3A4 and resid 31 and name CA)	5.34	0.15	0.15
	assign	(segid 3A4 and resid 21 and name N)	(segid 3A4 and resid 31 and name CB)	5.46	0.14	0.14
20	assign	(segid 3A4 and resid 21 and name N)	(segid 3A4 and resid 31 and name N)	6.69	0.15	0.16
	assign	(segid 3A4 and resid 21 and name N)	(segid 3A4 and resid 31 and name O)	6.37	0.17	0.17
	assign	(segid 3A4 and resid 21 and name N)	(segid 3A4 and resid 32 and name C)	4.38	0.23	0.23
	assign	(segid 3A4 and resid 21 and name N)	(segid 3A4 and resid 32 and name CA)	4.89	0.16	0.15
	assign	(segid 3A4 and resid 21 and name N)	(segid 3A4 and resid 32 and name CB)	5.12	0.17	0.16
25	assign	(segid 3A4 and resid 21 and name N)	(segid 3A4 and resid 32 and name N)	4.37	0.11	0.11
	assign	(segid 3A4 and resid 21 and name N)	(segid 3A4 and resid 32 and name O)	3.30	0.31	0.32
	assign	(segid 3A4 and resid 21 and name N)	(segid 3A4 and resid 33 and name C)	6.53	0.29	0.28
	assign	(segid 3A4 and resid 21 and name N)	(segid 3A4 and resid 33 and name CA)	5.73	0.30	0.29
	assign	(segid 3A4 and resid 21 and name N)	(segid 3A4 and resid 33 and name CB)	6.83	0.34	0.34
30	assign	(segid 3A4 and resid 21 and name N)	(segid 3A4 and resid 33 and name N)	5.43	0.23	0.24
	assign	(segid 3A4 and resid 21 and name N)	(segid 3A4 and resid 34 and name CA)	7.41	0.31	0.30
	assign	(segid 3A4 and resid 21 and name N)	(segid 3A4 and resid 34 and name CB)	6.99	0.34	0.34
	assign	(segid 3A4 and resid 21 and name N)	(segid 3A4 and resid 34 and name N)	6.40	0.30	0.29
	assign	(segid 3A4 and resid 21 and name O)	(segid 3A4 and resid 31 and name CB)	3.32	0.09	0.09
35	assign	(segid 3A4 and resid 21 and name O)	(segid 3A4 and resid 22 and name C)	3.59	0.23	0.23
	assign	(segid 3A4 and resid 21 and name O)	(segid 3A4 and resid 22 and name CA)	2.79	0.06	0.06
	assign	(segid 3A4 and resid 21 and name O)	(segid 3A4 and resid 22 and name N)	2.26	0.01	0.02
	assign	(segid 3A4 and resid 21 and name O)	(segid 3A4 and resid 22 and name O)	4.23	0.32	0.32
	assign	(segid 3A4 and resid 21 and name O)	(segid 3A4 and resid 23 and name C)	6.43	0.28	0.28
40	assign	(segid 3A4 and resid 21 and name O)	(segid 3A4 and resid 23 and name CA)	5.34	0.33	0.34
	assign	(segid 3A4 and resid 21 and name O)	(segid 3A4 and resid 23 and name CB)	5.54	0.46	0.45
	assign	(segid 3A4 and resid 21 and name O)	(segid 3A4 and resid 23 and name N)	4.12	0.25	0.26
	assign	(segid 3A4 and resid 21 and name O)	(segid 3A4 and resid 23 and name O)	6.40	0.19	0.19
	assign	(segid 3A4 and resid 21 and name O)	(segid 3A4 and resid 30 and name C)	4.66	0.17	0.17
45	assign	(segid 3A4 and resid 21 and name O)	(segid 3A4 and resid 30 and name CA)	6.15	0.18	0.18
	assign	(segid 3A4 and resid 21 and name O)	(segid 3A4 and resid 30 and name N)	6.60	0.18	0.17
	assign	(segid 3A4 and resid 21 and name O)	(segid 3A4 and resid 30 and name O)	4.03	0.24	0.24
	assign	(segid 3A4 and resid 21 and name O)	(segid 3A4 and resid 31 and name C)	3.47	0.07	0.07
	assign	(segid 3A4 and resid 21 and name O)	(segid 3A4 and resid 31 and name CA)	3.27	0.12	0.12
50	assign	(segid 3A4 and resid 21 and name O)	(segid 3A4 and resid 31 and name CB)	3.94	0.19	0.19
	assign	(segid 3A4 and resid 21 and name O)	(segid 3A4 and resid 31 and name N)	4.42	0.11	0.11
	assign	(segid 3A4 and resid 21 and name O)	(segid 3A4 and resid 31 and name O)	4.67	0.07	0.07
	assign	(segid 3A4 and resid 21 and name O)	(segid 3A4 and resid 32 and name C)	4.21	0.24	0.23
	assign	(segid 3A4 and resid 21 and name O)	(segid 3A4 and resid 32 and name CA)	3.85	0.20	0.19
55	assign	(segid 3A4 and resid 21 and name O)	(segid 3A4 and resid 32 and name CB)	4.05	0.22	0.23
	assign	(segid 3A4 and resid 21 and name O)	(segid 3A4 and resid 32 and name N)	2.80	0.13	0.13
	assign	(segid 3A4 and resid 21 and name O)	(segid 3A4 and resid 32 and name O)	3.71	0.32	0.31
	assign	(segid 3A4 and resid 21 and name O)	(segid 3A4 and resid 33 and name C)	7.23	0.22	0.23
	assign	(segid 3A4 and resid 21 and name O)	(segid 3A4 and resid 33 and name CA)	6.32	0.22	0.21
60	assign	(segid 3A4 and resid 21 and name O)	(segid 3A4 and resid 33 and name CB)	7.34	0.22	0.22
	assign	(segid 3A4 and resid 21 and name O)	(segid 3A4 and resid 33 and name N)	5.44	0.19	0.19
	assign	(segid 3A4 and resid 21 and name O)	(segid 3A4 and resid 342 and name O)	7.23	0.12	0.13
	assign	(segid 3A4 and resid 21 and name O)	(segid 3A4 and resid 344 and name N)	7.44	0.13	0.12
	assign	(segid 3A4 and resid 21 and name O)	(segid 3A4 and resid 344 and name O)	7.21	0.30	0.29
65	assign	(segid 3A4 and resid 220 and name C)	(segid 3A4 and resid 220 and name CB)	2.52	0.02	0.01
	assign	(segid 3A4 and resid 220 and name C)	(segid 3A4 and resid 220 and name O)	1.24	0.01	0.00
	assign	(segid 3A4 and resid 220 and name C)	(segid 3A4 and resid 221 and name C)	3.01	0.06	0.05
	assign	(segid 3A4 and resid 220 and name C)	(segid 3A4 and resid 221 and name CA)	2.43	0.01	0.00
	assign	(segid 3A4 and resid 220 and name C)	(segid 3A4 and resid 221 and name CB)	3.71	0.02	0.02
70	assign	(segid 3A4 and resid 220 and name C)	(segid 3A4 and resid 221 and name N)	1.32	0.02	0.02
	assign	(segid 3A4 and resid 220 and name C)	(segid 3A4 and resid 221 and name O)	3.78	0.09	0.09
	assign	(segid 3A4 and resid 220 and name C)	(segid 3A4 and resid 222 and name C)	4.53	0.06	0.06
	assign	(segid 3A4 and resid 220 and name C)	(segid 3A4 and resid 222 and name CA)	4.48	0.05	0.06
	assign	(segid 3A4 and resid 220 and name C)	(segid 3A4 and resid 222 and name CB)	5.24	0.09	0.09
75	assign	(segid 3A4 and resid 220 and name C)	(segid 3A4 and resid 222 and name N)	3.32	0.05	0.05
	assign	(segid 3A4 and resid 220 and name C)	(segid 3A4 and resid 222 and name O)	5.62	0.07	0.06
	assign	(segid 3A4 and resid 220 and name C)	(segid 3A4 and resid 223 and name C)	4.82	0.06	0.05
	assign	(segid 3A4 and resid 220 and name C)	(segid 3A4 and resid 223 and name CA)	4.48	0.05	0.05
	assign	(segid 3A4 and resid 220 and name C)	(segid 3A4 and resid 223 and name CB)	4.25	0.08	0.07
80	assign	(segid 3A4 and resid 220 and name C)	(segid 3A4 and resid 223 and name N)	3.77	0.06	0.06
	assign	(segid 3A4 and resid 220 and name C)	(segid 3A4 and resid 223 and name O)	6.02	0.06	0.07
	assign	(segid 3A4 and resid 220 and name C)	(segid 3A4 and resid 224 and name C)	6.08	0.08	0.09
	assign	(segid 3A4 and resid 220 and name C)	(segid 3A4 and resid 224 and name CA)	5.05	0.05	0.05

5	assign	(segid 3A4 and resid 220 and name C)	(segid 3A4 and resid 224 and name CB)	4.71	0.08	0.07
	assign	(segid 3A4 and resid 220 and name C)	(segid 3A4 and resid 224 and name N)	4.11	0.04	0.04
	assign	(segid 3A4 and resid 220 and name C)	(segid 3A4 and resid 224 and name O)	7.23	0.09	0.10
	assign	(segid 3A4 and resid 220 and name C)	(segid 3A4 and resid 225 and name CA)	7.18	0.12	0.13
	assign	(segid 3A4 and resid 220 and name C)	(segid 3A4 and resid 225 and name CB)	7.17	0.16	0.17
10	assign	(segid 3A4 and resid 220 and name C)	(segid 3A4 and resid 225 and name N)	5.94	0.11	0.11
	assign	(segid 3A4 and resid 220 and name CA)	(segid 3A4 and resid 220 and name C)	1.53	0.01	0.00
	assign	(segid 3A4 and resid 220 and name CA)	(segid 3A4 and resid 220 and name CB)	1.53	0.01	0.01
	assign	(segid 3A4 and resid 220 and name CA)	(segid 3A4 and resid 220 and name O)	2.39	0.01	0.01
	assign	(segid 3A4 and resid 220 and name CA)	(segid 3A4 and resid 221 and name C)	4.42	0.04	0.05
15	assign	(segid 3A4 and resid 220 and name CA)	(segid 3A4 and resid 221 and name CA)	3.82	0.01	0.01
	assign	(segid 3A4 and resid 220 and name CA)	(segid 3A4 and resid 221 and name CB)	4.89	0.02	0.02
	assign	(segid 3A4 and resid 220 and name CA)	(segid 3A4 and resid 221 and name N)	2.46	0.02	0.01
	assign	(segid 3A4 and resid 220 and name CA)	(segid 3A4 and resid 221 and name O)	5.26	0.09	0.08
	assign	(segid 3A4 and resid 220 and name CA)	(segid 3A4 and resid 222 and name C)	5.52	0.05	0.06
20	assign	(segid 3A4 and resid 220 and name CA)	(segid 3A4 and resid 222 and name CA)	5.52	0.04	0.04
	assign	(segid 3A4 and resid 220 and name CA)	(segid 3A4 and resid 222 and name CB)	5.95	0.10	0.11
	assign	(segid 3A4 and resid 220 and name CA)	(segid 3A4 and resid 222 and name N)	4.46	0.05	0.04
	assign	(segid 3A4 and resid 220 and name CA)	(segid 3A4 and resid 222 and name O)	6.65	0.06	0.07
	assign	(segid 3A4 and resid 220 and name CA)	(segid 3A4 and resid 223 and name C)	5.66	0.08	0.09
25	assign	(segid 3A4 and resid 220 and name CA)	(segid 3A4 and resid 223 and name CA)	5.08	0.05	0.06
	assign	(segid 3A4 and resid 220 and name CA)	(segid 3A4 and resid 223 and name CB)	4.41	0.09	0.09
	assign	(segid 3A4 and resid 220 and name CA)	(segid 3A4 and resid 223 and name N)	4.55	0.05	0.05
	assign	(segid 3A4 and resid 220 and name CA)	(segid 3A4 and resid 223 and name O)	6.83	0.09	0.10
	assign	(segid 3A4 and resid 220 and name CA)	(segid 3A4 and resid 224 and name C)	7.36	0.11	0.10
30	assign	(segid 3A4 and resid 220 and name CA)	(segid 3A4 and resid 224 and name CA)	6.18	0.07	0.08
	assign	(segid 3A4 and resid 220 and name CA)	(segid 3A4 and resid 224 and name CB)	5.90	0.10	0.10
	assign	(segid 3A4 and resid 220 and name CA)	(segid 3A4 and resid 224 and name N)	5.17	0.08	0.07
	assign	(segid 3A4 and resid 220 and name CA)	(segid 3A4 and resid 225 and name CA)	8.59	0.12	0.12
	assign	(segid 3A4 and resid 220 and name CA)	(segid 3A4 and resid 225 and name CB)	8.61	0.15	0.15
35	assign	(segid 3A4 and resid 220 and name CA)	(segid 3A4 and resid 225 and name N)	7.31	0.11	0.12
	assign	(segid 3A4 and resid 220 and name CA)	(segid 3A4 and resid 226 and name CA)	10.11	0.11	0.10
	assign	(segid 3A4 and resid 220 and name CA)	(segid 3A4 and resid 240 and name CA)	15.24	0.70	0.70
	assign	(segid 3A4 and resid 220 and name CA)	(segid 3A4 and resid 240 and name CB)	16.49	0.69	0.68
	assign	(segid 3A4 and resid 220 and name CA)	(segid 3A4 and resid 241 and name CA)	14.19	0.73	0.73
40	assign	(segid 3A4 and resid 220 and name CA)	(segid 3A4 and resid 241 and name CB)	15.12	0.80	0.79
	assign	(segid 3A4 and resid 220 and name CA)	(segid 3A4 and resid 242 and name CA)	15.54	0.68	0.67
	assign	(segid 3A4 and resid 220 and name CA)	(segid 3A4 and resid 242 and name CB)	16.97	0.64	0.65
	assign	(segid 3A4 and resid 220 and name CA)	(segid 3A4 and resid 243 and name CA)	13.70	0.51	0.50
	assign	(segid 3A4 and resid 220 and name CA)	(segid 3A4 and resid 243 and name CB)	13.91	0.48	0.48
45	assign	(segid 3A4 and resid 220 and name CA)	(segid 3A4 and resid 244 and name CA)	10.28	0.57	0.57
	assign	(segid 3A4 and resid 220 and name CA)	(segid 3A4 and resid 244 and name CB)	10.06	0.62	0.62
	assign	(segid 3A4 and resid 220 and name CA)	(segid 3A4 and resid 245 and name CA)	11.70	0.57	0.57
	assign	(segid 3A4 and resid 220 and name CA)	(segid 3A4 and resid 245 and name CB)	13.06	0.57	0.57
	assign	(segid 3A4 and resid 220 and name CA)	(segid 3A4 and resid 246 and name CA)	13.14	0.44	0.44
50	assign	(segid 3A4 and resid 220 and name CA)	(segid 3A4 and resid 246 and name CB)	14.22	0.51	0.51
	assign	(segid 3A4 and resid 220 and name CA)	(segid 3A4 and resid 247 and name CA)	10.19	0.45	0.45
	assign	(segid 3A4 and resid 220 and name CA)	(segid 3A4 and resid 247 and name CB)	9.38	0.51	0.52
	assign	(segid 3A4 and resid 220 and name CA)	(segid 3A4 and resid 248 and name CA)	8.49	0.33	0.33
	assign	(segid 3A4 and resid 220 and name CA)	(segid 3A4 and resid 248 and name CB)	8.35	0.43	0.43
55	assign	(segid 3A4 and resid 220 and name CA)	(segid 3A4 and resid 249 and name CA)	12.02	0.30	0.30
	assign	(segid 3A4 and resid 220 and name CA)	(segid 3A4 and resid 250 and name CA)	12.50	0.34	0.35
	assign	(segid 3A4 and resid 220 and name CA)	(segid 3A4 and resid 250 and name CB)	12.64	0.50	0.50
	assign	(segid 3A4 and resid 220 and name CA)	(segid 3A4 and resid 251 and name CA)	9.78	0.34	0.34
	assign	(segid 3A4 and resid 220 and name CA)	(segid 3A4 and resid 251 and name CB)	8.28	0.33	0.34
60	assign	(segid 3A4 and resid 220 and name CA)	(segid 3A4 and resid 252 and name CA)	11.34	0.46	0.46
	assign	(segid 3A4 and resid 220 and name CA)	(segid 3A4 and resid 252 and name CB)	11.54	0.45	0.45
	assign	(segid 3A4 and resid 220 and name CA)	(segid 3A4 and resid 253 and name CA)	14.79	0.39	0.39
	assign	(segid 3A4 and resid 220 and name CA)	(segid 3A4 and resid 254 and name CA)	14.78	0.65	0.65
	assign	(segid 3A4 and resid 220 and name CA)	(segid 3A4 and resid 255 and name CA)	13.53	1.19	1.18
65	assign	(segid 3A4 and resid 220 and name CA)	(segid 3A4 and resid 256 and name CA)	15.54	0.47	0.46
	assign	(segid 3A4 and resid 220 and name CA)	(segid 3A4 and resid 259 and name CA)	18.63	0.44	0.44
	assign	(segid 3A4 and resid 220 and name CA)	(segid 3A4 and resid 259 and name CB)	17.33	0.42	0.43
	assign	(segid 3A4 and resid 220 and name CA)	(segid 3A4 and resid 391 and name CA)	16.69	0.43	0.43
	assign	(segid 3A4 and resid 220 and name CA)	(segid 3A4 and resid 391 and name CB)	17.10	0.42	0.42
70	assign	(segid 3A4 and resid 220 and name CA)	(segid 3A4 and resid 392 and name CA)	13.40	0.40	0.41
	assign	(segid 3A4 and resid 220 and name CA)	(segid 3A4 and resid 392 and name CB)	12.40	0.35	0.35
	assign	(segid 3A4 and resid 220 and name CA)	(segid 3A4 and resid 393 and name CA)	12.65	0.42	0.42
	assign	(segid 3A4 and resid 220 and name CA)	(segid 3A4 and resid 394 and name CA)	16.13	0.45	0.45
	assign	(segid 3A4 and resid 220 and name CA)	(segid 3A4 and resid 394 and name CB)	17.12	0.46	0.45
75	assign	(segid 3A4 and resid 220 and name CA)	(segid 3A4 and resid 395 and name CA)	15.40	0.57	0.58
	assign	(segid 3A4 and resid 220 and name CA)	(segid 3A4 and resid 396 and name CA)	13.27	0.66	0.65
	assign	(segid 3A4 and resid 220 and name CA)	(segid 3A4 and resid 396 and name CB)	11.88	0.62	0.63
	assign	(segid 3A4 and resid 220 and name CA)	(segid 3A4 and resid 397 and name CA)	15.98	0.58	0.58
	assign	(segid 3A4 and resid 220 and name CA)	(segid 3A4 and resid 397 and name CB)	16.47	0.54	0.53
80	assign	(segid 3A4 and resid 220 and name CA)	(segid 3A4 and resid 398 and name CA)	18.76	0.61	0.61
	assign	(segid 3A4 and resid 220 and name CA)	(segid 3A4 and resid 399 and name CA)	17.57	0.67	0.67
	assign	(segid 3A4 and resid 220 and name CA)	(segid 3A4 and resid 399 and name CB)	16.36	0.67	0.68
	assign	(segid 3A4 and resid 220 and name CA)	(segid 3A4 and resid 400 and name CA)	17.33	0.75	0.75
	assign	(segid 3A4 and resid 220 and name CA)	(segid 3A4 and resid 400 and name CB)	16.45	0.79	0.79
	assign	(segid 3A4 and resid 220 and name C)	(segid 3A4 and resid 221 and name C)	5.45	0.09	0.09
	assign	(segid 3A4 and resid 220 and name CB)	(segid 3A4 and resid 221 and name CA)	4.51	0.09	0.09
	assign	(segid 3A4 and resid 220 and name CB)	(segid 3A4 and resid 221 and name CB)	5.40	0.10	0.11

	assign (segid 3A4 and resid 220 and name CB)	(segid 3A4 and resid 221 and name N)	3.20	0.11	0.11
	assign (segid 3A4 and resid 220 and name CB)	(segid 3A4 and resid 221 and name O)	6.22	0.11	0.11
	assign (segid 3A4 and resid 220 and name CB)	(segid 3A4 and resid 222 and name C)	6.90	0.07	0.07
	assign (segid 3A4 and resid 220 and name CB)	(segid 3A4 and resid 222 and name CA)	6.89	0.06	0.06
5	assign (segid 3A4 and resid 220 and name CB)	(segid 3A4 and resid 222 and name CB)	7.41	0.13	0.12
	assign (segid 3A4 and resid 220 and name CB)	(segid 3A4 and resid 222 and name N)	5.71	0.06	0.06
	assign (segid 3A4 and resid 220 and name CB)	(segid 3A4 and resid 223 and name C)	6.73	0.14	0.13
	assign (segid 3A4 and resid 220 and name CB)	(segid 3A4 and resid 223 and name CA)	6.35	0.08	0.09
	assign (segid 3A4 and resid 220 and name CB)	(segid 3A4 and resid 223 and name CB)	5.57	0.11	0.11
	assign (segid 3A4 and resid 220 and name CB)	(segid 3A4 and resid 223 and name N)	5.94	0.07	0.07
10	assign (segid 3A4 and resid 220 and name CB)	(segid 3A4 and resid 224 and name CA)	6.85	0.10	0.10
	assign (segid 3A4 and resid 220 and name CB)	(segid 3A4 and resid 224 and name CB)	6.29	0.11	0.11
	assign (segid 3A4 and resid 220 and name CB)	(segid 3A4 and resid 224 and name N)	6.07	0.10	0.10
	assign (segid 3A4 and resid 220 and name CB)	(segid 3A4 and resid 225 and name CA)	9.52	0.14	0.14
	assign (segid 3A4 and resid 220 and name CB)	(segid 3A4 and resid 225 and name CB)	9.62	0.18	0.17
15	assign (segid 3A4 and resid 220 and name CB)	(segid 3A4 and resid 226 and name CA)	11.28	0.10	0.10
	assign (segid 3A4 and resid 220 and name CB)	(segid 3A4 and resid 240 and name CA)	15.46	0.82	0.82
	assign (segid 3A4 and resid 220 and name CB)	(segid 3A4 and resid 240 and name CB)	16.62	0.82	0.82
	assign (segid 3A4 and resid 220 and name CB)	(segid 3A4 and resid 241 and name CA)	14.38	0.86	0.87
	assign (segid 3A4 and resid 220 and name CB)	(segid 3A4 and resid 241 and name CB)	15.36	0.92	0.92
20	assign (segid 3A4 and resid 220 and name CB)	(segid 3A4 and resid 242 and name CA)	15.37	0.83	0.82
	assign (segid 3A4 and resid 220 and name CB)	(segid 3A4 and resid 242 and name CB)	16.78	0.80	0.80
	assign (segid 3A4 and resid 220 and name CB)	(segid 3A4 and resid 243 and name CA)	13.40	0.67	0.67
	assign (segid 3A4 and resid 220 and name CB)	(segid 3A4 and resid 243 and name CB)	13.69	0.64	0.64
	assign (segid 3A4 and resid 220 and name CB)	(segid 3A4 and resid 244 and name CA)	10.13	0.76	0.76
25	assign (segid 3A4 and resid 220 and name CB)	(segid 3A4 and resid 244 and name CB)	10.12	0.80	0.80
	assign (segid 3A4 and resid 220 and name CB)	(segid 3A4 and resid 245 and name CA)	11.31	0.79	0.79
	assign (segid 3A4 and resid 220 and name CB)	(segid 3A4 and resid 245 and name CB)	12.72	0.80	0.80
	assign (segid 3A4 and resid 220 and name CB)	(segid 3A4 and resid 246 and name CA)	12.41	0.62	0.62
	assign (segid 3A4 and resid 220 and name CB)	(segid 3A4 and resid 246 and name CB)	13.51	0.68	0.68
30	assign (segid 3A4 and resid 220 and name CB)	(segid 3A4 and resid 247 and name CA)	9.33	0.61	0.61
	assign (segid 3A4 and resid 220 and name CB)	(segid 3A4 and resid 247 and name CB)	8.65	0.67	0.66
	assign (segid 3A4 and resid 220 and name CB)	(segid 3A4 and resid 248 and name CA)	7.60	0.51	0.50
	assign (segid 3A4 and resid 220 and name CB)	(segid 3A4 and resid 248 and name CB)	7.66	0.61	0.60
	assign (segid 3A4 and resid 220 and name CB)	(segid 3A4 and resid 249 and name CA)	10.99	0.41	0.40
35	assign (segid 3A4 and resid 220 and name CB)	(segid 3A4 and resid 250 and name CA)	11.25	0.39	0.39
	assign (segid 3A4 and resid 220 and name CB)	(segid 3A4 and resid 250 and name CB)	11.41	0.55	0.56
	assign (segid 3A4 and resid 220 and name CB)	(segid 3A4 and resid 251 and name CA)	8.38	0.32	0.32
	assign (segid 3A4 and resid 220 and name CB)	(segid 3A4 and resid 251 and name CB)	6.90	0.32	0.32
	assign (segid 3A4 and resid 220 and name CB)	(segid 3A4 and resid 251 and name CG)	6.53	0.36	0.36
40	assign (segid 3A4 and resid 220 and name CB)	(segid 3A4 and resid 252 and name CA)	10.03	0.39	0.39
	assign (segid 3A4 and resid 220 and name CB)	(segid 3A4 and resid 252 and name CB)	10.34	0.38	0.38
	assign (segid 3A4 and resid 220 and name CB)	(segid 3A4 and resid 253 and name CA)	13.42	0.33	0.33
	assign (segid 3A4 and resid 220 and name CB)	(segid 3A4 and resid 254 and name CA)	13.30	0.64	0.65
	assign (segid 3A4 and resid 220 and name CB)	(segid 3A4 and resid 255 and name CA)	12.06	1.16	1.16
45	assign (segid 3A4 and resid 220 and name CB)	(segid 3A4 and resid 256 and name CA)	14.15	0.44	0.43
	assign (segid 3A4 and resid 220 and name CB)	(segid 3A4 and resid 257 and name CA)	17.55	0.65	0.65
	assign (segid 3A4 and resid 220 and name CB)	(segid 3A4 and resid 258 and name CA)	17.99	0.71	0.71
	assign (segid 3A4 and resid 220 and name CB)	(segid 3A4 and resid 258 and name CB)	17.29	0.80	0.80
	assign (segid 3A4 and resid 220 and name CB)	(segid 3A4 and resid 259 and name CA)	17.24	0.45	0.45
50	assign (segid 3A4 and resid 220 and name CB)	(segid 3A4 and resid 259 and name CB)	15.97	0.43	0.43
	assign (segid 3A4 and resid 220 and name CB)	(segid 3A4 and resid 384 and name CB)	19.11	0.44	0.45
	assign (segid 3A4 and resid 220 and name CB)	(segid 3A4 and resid 389 and name CA)	18.47	0.40	0.41
	assign (segid 3A4 and resid 220 and name CB)	(segid 3A4 and resid 389 and name CB)	19.16	0.43	0.44
	assign (segid 3A4 and resid 220 and name CB)	(segid 3A4 and resid 390 and name CA)	18.26	0.43	0.42
55	assign (segid 3A4 and resid 220 and name CB)	(segid 3A4 and resid 390 and name CB)	18.80	0.44	0.43
	assign (segid 3A4 and resid 220 and name CB)	(segid 3A4 and resid 391 and name CA)	15.41	0.45	0.45
	assign (segid 3A4 and resid 220 and name CB)	(segid 3A4 and resid 391 and name CB)	15.78	0.44	0.43
	assign (segid 3A4 and resid 220 and name CB)	(segid 3A4 and resid 392 and name CA)	12.23	0.39	0.40
	assign (segid 3A4 and resid 220 and name CB)	(segid 3A4 and resid 392 and name CB)	11.24	0.35	0.36
60	assign (segid 3A4 and resid 220 and name CB)	(segid 3A4 and resid 393 and name CA)	11.36	0.42	0.42
	assign (segid 3A4 and resid 220 and name CB)	(segid 3A4 and resid 394 and name CA)	14.92	0.44	0.44
	assign (segid 3A4 and resid 220 and name CB)	(segid 3A4 and resid 394 and name CB)	15.94	0.42	0.42
	assign (segid 3A4 and resid 220 and name CB)	(segid 3A4 and resid 395 and name CA)	14.40	0.53	0.54
	assign (segid 3A4 and resid 220 and name CB)	(segid 3A4 and resid 396 and name CA)	12.20	0.64	0.64
65	assign (segid 3A4 and resid 220 and name CB)	(segid 3A4 and resid 396 and name CB)	10.77	0.62	0.63
	assign (segid 3A4 and resid 220 and name CB)	(segid 3A4 and resid 397 and name CA)	14.74	0.54	0.54
	assign (segid 3A4 and resid 220 and name CB)	(segid 3A4 and resid 397 and name CB)	15.17	0.50	0.49
	assign (segid 3A4 and resid 220 and name CB)	(segid 3A4 and resid 398 and name CA)	17.65	0.57	0.57
	assign (segid 3A4 and resid 220 and name CB)	(segid 3A4 and resid 398 and name CB)	18.17	0.54	0.54
70	assign (segid 3A4 and resid 220 and name CB)	(segid 3A4 and resid 399 and name CA)	16.65	0.61	0.61
	assign (segid 3A4 and resid 220 and name CB)	(segid 3A4 and resid 399 and name CB)	15.51	0.62	0.62
	assign (segid 3A4 and resid 220 and name CB)	(segid 3A4 and resid 400 and name CA)	16.31	0.67	0.67
	assign (segid 3A4 and resid 220 and name CB)	(segid 3A4 and resid 400 and name CB)	15.37	0.72	0.71
	assign (segid 3A4 and resid 220 and name CB)	(segid 3A4 and resid 403 and name CB)	19.25	0.62	0.61
75	assign (segid 3A4 and resid 220 and name CB)	(segid 3A4 and resid 403 and name C)	2.49	0.02	0.03
	assign (segid 3A4 and resid 220 and name N)	(segid 3A4 and resid 220 and name CA)	1.46	0.01	0.01
	assign (segid 3A4 and resid 220 and name N)	(segid 3A4 and resid 220 and name CB)	2.45	0.02	0.03
	assign (segid 3A4 and resid 220 and name N)	(segid 3A4 and resid 220 and name O)	3.52	0.05	0.04
	assign (segid 3A4 and resid 220 and name N)	(segid 3A4 and resid 221 and name C)	4.83	0.03	0.02
80	assign (segid 3A4 and resid 220 and name N)	(segid 3A4 and resid 221 and name CA)	4.30	0.05	0.05
	assign (segid 3A4 and resid 220 and name N)	(segid 3A4 and resid 221 and name CB)	5.07	0.07	0.07
	assign (segid 3A4 and resid 220 and name N)	(segid 3A4 and resid 221 and name N)	2.89	0.06	0.07

	assign (segid 3A4 and resid 221 and name CA)	(segid 3A4 and resid 225 and name CA)	6.04	0.14	0.13
	assign (segid 3A4 and resid 221 and name CA)	(segid 3A4 and resid 225 and name CB)	5.69	0.19	0.18
	assign (segid 3A4 and resid 221 and name CA)	(segid 3A4 and resid 225 and name N)	5.10	0.10	0.09
	assign (segid 3A4 and resid 221 and name CA)	(segid 3A4 and resid 226 and name CA)	8.63	0.19	0.19
	assign (segid 3A4 and resid 221 and name CA)	(segid 3A4 and resid 226 and name N)	7.30	0.16	0.17
5	assign (segid 3A4 and resid 221 and name CA)	(segid 3A4 and resid 240 and name CA)	12.72	0.68	0.68
	assign (segid 3A4 and resid 221 and name CA)	(segid 3A4 and resid 240 and name CB)	14.00	0.64	0.64
	assign (segid 3A4 and resid 221 and name CA)	(segid 3A4 and resid 241 and name CA)	11.09	0.74	0.73
	assign (segid 3A4 and resid 221 and name CA)	(segid 3A4 and resid 241 and name CB)	11.81	0.80	0.81
	assign (segid 3A4 and resid 221 and name CA)	(segid 3A4 and resid 242 and name CA)	12.79	0.63	0.64
10	assign (segid 3A4 and resid 221 and name CA)	(segid 3A4 and resid 242 and name CB)	14.29	0.62	0.62
	assign (segid 3A4 and resid 221 and name CA)	(segid 3A4 and resid 243 and name CA)	11.70	0.39	0.38
	assign (segid 3A4 and resid 221 and name CA)	(segid 3A4 and resid 243 and name CB)	12.10	0.38	0.38
	assign (segid 3A4 and resid 221 and name CA)	(segid 3A4 and resid 244 and name CA)	7.97	0.43	0.44
	assign (segid 3A4 and resid 221 and name CA)	(segid 3A4 and resid 244 and name CB)	7.38	0.54	0.54
15	assign (segid 3A4 and resid 221 and name CA)	(segid 3A4 and resid 245 and name CA)	9.16	0.34	0.34
	assign (segid 3A4 and resid 221 and name CA)	(segid 3A4 and resid 245 and name CB)	10.31	0.35	0.36
	assign (segid 3A4 and resid 221 and name CA)	(segid 3A4 and resid 246 and name CA)	11.48	0.31	0.31
	assign (segid 3A4 and resid 221 and name CA)	(segid 3A4 and resid 246 and name CB)	12.60	0.31	0.32
20	assign (segid 3A4 and resid 221 and name CA)	(segid 3A4 and resid 247 and name CA)	9.41	0.29	0.29
	assign (segid 3A4 and resid 221 and name CA)	(segid 3A4 and resid 247 and name CB)	8.69	0.27	0.27
	assign (segid 3A4 and resid 221 and name CA)	(segid 3A4 and resid 248 and name CA)	7.37	0.50	0.51
	assign (segid 3A4 and resid 221 and name CA)	(segid 3A4 and resid 248 and name CB)	6.64	0.54	0.53
	assign (segid 3A4 and resid 221 and name CA)	(segid 3A4 and resid 249 and name CA)	10.95	0.58	0.57
	assign (segid 3A4 and resid 221 and name CA)	(segid 3A4 and resid 250 and name CA)	12.41	0.61	0.60
25	assign (segid 3A4 and resid 221 and name CA)	(segid 3A4 and resid 250 and name CB)	12.61	0.56	0.56
	assign (segid 3A4 and resid 221 and name CA)	(segid 3A4 and resid 251 and name CA)	10.55	0.77	0.77
	assign (segid 3A4 and resid 221 and name CA)	(segid 3A4 and resid 251 and name CB)	9.16	0.77	0.76
	assign (segid 3A4 and resid 221 and name CA)	(segid 3A4 and resid 252 and name CA)	11.61	0.95	0.96
	assign (segid 3A4 and resid 221 and name CA)	(segid 3A4 and resid 252 and name CB)	11.35	0.94	0.93
30	assign (segid 3A4 and resid 221 and name CA)	(segid 3A4 and resid 253 and name CA)	15.03	0.81	0.81
	assign (segid 3A4 and resid 221 and name CA)	(segid 3A4 and resid 254 and name CA)	15.80	0.93	0.94
	assign (segid 3A4 and resid 221 and name CA)	(segid 3A4 and resid 255 and name CA)	15.07	1.44	1.44
	assign (segid 3A4 and resid 221 and name CA)	(segid 3A4 and resid 256 and name CA)	16.73	0.81	0.81
	assign (segid 3A4 and resid 221 and name CA)	(segid 3A4 and resid 391 and name CA)	18.99	0.41	0.41
35	assign (segid 3A4 and resid 221 and name CA)	(segid 3A4 and resid 392 and name CA)	15.93	0.27	0.28
	assign (segid 3A4 and resid 221 and name CA)	(segid 3A4 and resid 392 and name CB)	14.74	0.26	0.25
	assign (segid 3A4 and resid 221 and name CA)	(segid 3A4 and resid 393 and name CA)	15.44	0.39	0.40
	assign (segid 3A4 and resid 221 and name CA)	(segid 3A4 and resid 394 and name CA)	19.12	0.41	0.42
40	assign (segid 3A4 and resid 221 and name CA)	(segid 3A4 and resid 395 and name CA)	18.81	0.54	0.54
	assign (segid 3A4 and resid 221 and name CA)	(segid 3A4 and resid 396 and name CA)	16.56	0.61	0.61
	assign (segid 3A4 and resid 221 and name CA)	(segid 3A4 and resid 396 and name CB)	15.11	0.59	0.59
	assign (segid 3A4 and resid 221 and name CA)	(segid 3A4 and resid 397 and name CA)	18.91	0.50	0.49
	assign (segid 3A4 and resid 221 and name CA)	(segid 3A4 and resid 222 and name C)	5.44	0.06	0.06
45	assign (segid 3A4 and resid 221 and name CB)	(segid 3A4 and resid 222 and name CA)	4.51	0.07	0.08
	assign (segid 3A4 and resid 221 and name CB)	(segid 3A4 and resid 222 and name CB)	5.42	0.14	0.13
	assign (segid 3A4 and resid 221 and name CB)	(segid 3A4 and resid 222 and name N)	3.19	0.09	0.08
	assign (segid 3A4 and resid 221 and name CB)	(segid 3A4 and resid 222 and name O)	6.32	0.09	0.08
	assign (segid 3A4 and resid 221 and name CB)	(segid 3A4 and resid 223 and name C)	6.86	0.06	0.06
	assign (segid 3A4 and resid 221 and name CB)	(segid 3A4 and resid 223 and name CA)	6.80	0.07	0.06
50	assign (segid 3A4 and resid 221 and name CB)	(segid 3A4 and resid 223 and name CB)	7.26	0.09	0.09
	assign (segid 3A4 and resid 221 and name CB)	(segid 3A4 and resid 223 and name N)	5.61	0.07	0.06
	assign (segid 3A4 and resid 221 and name CB)	(segid 3A4 and resid 224 and name C)	6.78	0.04	0.04
	assign (segid 3A4 and resid 221 and name CB)	(segid 3A4 and resid 224 and name CA)	6.45	0.12	0.12
	assign (segid 3A4 and resid 221 and name CB)	(segid 3A4 and resid 224 and name CB)	5.80	0.21	0.22
55	assign (segid 3A4 and resid 221 and name CB)	(segid 3A4 and resid 224 and name N)	5.96	0.11	0.10
	assign (segid 3A4 and resid 221 and name CB)	(segid 3A4 and resid 225 and name CA)	6.78	0.13	0.13
	assign (segid 3A4 and resid 221 and name CB)	(segid 3A4 and resid 225 and name CB)	6.16	0.19	0.19
	assign (segid 3A4 and resid 221 and name CB)	(segid 3A4 and resid 225 and name N)	6.09	0.10	0.09
	assign (segid 3A4 and resid 221 and name CB)	(segid 3A4 and resid 226 and name CA)	9.61	0.22	0.21
60	assign (segid 3A4 and resid 221 and name CB)	(segid 3A4 and resid 240 and name CA)	13.14	0.72	0.73
	assign (segid 3A4 and resid 221 and name CB)	(segid 3A4 and resid 240 and name CB)	14.39	0.70	0.70
	assign (segid 3A4 and resid 221 and name CB)	(segid 3A4 and resid 241 and name CA)	11.10	0.80	0.81
	assign (segid 3A4 and resid 221 and name CB)	(segid 3A4 and resid 241 and name CB)	11.68	0.88	0.89
	assign (segid 3A4 and resid 221 and name CB)	(segid 3A4 and resid 242 and name CA)	12.75	0.76	0.76
65	assign (segid 3A4 and resid 221 and name CB)	(segid 3A4 and resid 242 and name CB)	14.26	0.76	0.75
	assign (segid 3A4 and resid 221 and name CB)	(segid 3A4 and resid 243 and name CA)	12.05	0.50	0.50
	assign (segid 3A4 and resid 221 and name CB)	(segid 3A4 and resid 243 and name CB)	12.62	0.49	0.49
	assign (segid 3A4 and resid 221 and name CB)	(segid 3A4 and resid 244 and name CA)	8.31	0.53	0.53
	assign (segid 3A4 and resid 221 and name CB)	(segid 3A4 and resid 244 and name CB)	7.67	0.61	0.62
70	assign (segid 3A4 and resid 221 and name CB)	(segid 3A4 and resid 245 and name CA)	8.88	0.45	0.46
	assign (segid 3A4 and resid 221 and name CB)	(segid 3A4 and resid 245 and name CB)	9.92	0.45	0.45
	assign (segid 3A4 and resid 221 and name CB)	(segid 3A4 and resid 246 and name CA)	11.47	0.44	0.44
	assign (segid 3A4 and resid 221 and name CB)	(segid 3A4 and resid 246 and name CB)	12.69	0.44	0.44
	assign (segid 3A4 and resid 221 and name CB)	(segid 3A4 and resid 247 and name CA)	9.78	0.39	0.38
75	assign (segid 3A4 and resid 221 and name CB)	(segid 3A4 and resid 247 and name CB)	9.27	0.33	0.32
	assign (segid 3A4 and resid 221 and name CB)	(segid 3A4 and resid 248 and name CA)	7.27	0.59	0.60
	assign (segid 3A4 and resid 221 and name CB)	(segid 3A4 and resid 248 and name CB)	6.32	0.61	0.61
	assign (segid 3A4 and resid 221 and name CB)	(segid 3A4 and resid 249 and name CA)	10.59	0.72	0.72
	assign (segid 3A4 and resid 221 and name CB)	(segid 3A4 and resid 250 and name CA)	12.46	0.74	0.73
80	assign (segid 3A4 and resid 221 and name CB)	(segid 3A4 and resid 250 and name CB)	12.82	0.65	0.65
	assign (segid 3A4 and resid 221 and name CB)	(segid 3A4 and resid 251 and name CA)	10.71	0.88	0.88
	assign (segid 3A4 and resid 221 and name CB)	(segid 3A4 and resid 251 and name CB)	9.40	0.84	0.85

5	assign	(segid 3A4 and resid 221 and name CB)	(segid 3A4 and resid 252 and name CA)	11.27	1.09	1.09
	assign	(segid 3A4 and resid 221 and name CB)	(segid 3A4 and resid 252 and name CB)	10.84	1.08	1.08
	assign	(segid 3A4 and resid 221 and name CB)	(segid 3A4 and resid 253 and name CA)	14.74	0.95	0.95
	assign	(segid 3A4 and resid 221 and name CB)	(segid 3A4 and resid 254 and name CA)	15.85	1.04	1.05
	assign	(segid 3A4 and resid 221 and name CB)	(segid 3A4 and resid 255 and name CA)	15.08	1.54	1.54
	assign	(segid 3A4 and resid 221 and name CB)	(segid 3A4 and resid 256 and name CA)	16.44	0.93	0.94
	assign	(segid 3A4 and resid 221 and name CB)	(segid 3A4 and resid 392 and name CA)	16.85	0.29	0.28
	assign	(segid 3A4 and resid 221 and name CB)	(segid 3A4 and resid 392 and name CB)	15.67	0.27	0.28
10	assign	(segid 3A4 and resid 221 and name CB)	(segid 3A4 and resid 393 and name CA)	16.14	0.40	0.41
	assign	(segid 3A4 and resid 221 and name CB)	(segid 3A4 and resid 396 and name CA)	17.13	0.59	0.60
	assign	(segid 3A4 and resid 221 and name CB)	(segid 3A4 and resid 396 and name CB)	15.66	0.57	0.57
	assign	(segid 3A4 and resid 221 and name N)	(segid 3A4 and resid 221 and name C)	2.46	0.01	0.02
	assign	(segid 3A4 and resid 221 and name N)	(segid 3A4 and resid 221 and name CA)	1.46	0.01	0.00
15	assign	(segid 3A4 and resid 221 and name N)	(segid 3A4 and resid 221 and name CB)	2.46	0.02	0.03
	assign	(segid 3A4 and resid 221 and name N)	(segid 3A4 and resid 221 and name O)	3.46	0.04	0.04
	assign	(segid 3A4 and resid 221 and name N)	(segid 3A4 and resid 222 and name C)	4.71	0.04	0.03
	assign	(segid 3A4 and resid 221 and name N)	(segid 3A4 and resid 222 and name CA)	4.25	0.04	0.03
	assign	(segid 3A4 and resid 221 and name N)	(segid 3A4 and resid 222 and name CB)	5.02	0.11	0.12
20	assign	(segid 3A4 and resid 221 and name N)	(segid 3A4 and resid 222 and name N)	2.85	0.04	0.05
	assign	(segid 3A4 and resid 221 and name N)	(segid 3A4 and resid 222 and name O)	5.80	0.05	0.06
	assign	(segid 3A4 and resid 221 and name N)	(segid 3A4 and resid 223 and name C)	5.57	0.03	0.03
	assign	(segid 3A4 and resid 221 and name N)	(segid 3A4 and resid 223 and name CA)	5.27	0.02	0.03
	assign	(segid 3A4 and resid 221 and name N)	(segid 3A4 and resid 223 and name CB)	5.31	0.08	0.08
25	assign	(segid 3A4 and resid 221 and name N)	(segid 3A4 and resid 223 and name N)	4.28	0.02	0.02
	assign	(segid 3A4 and resid 221 and name N)	(segid 3A4 and resid 223 and name O)	6.77	0.03	0.04
	assign	(segid 3A4 and resid 221 and name N)	(segid 3A4 and resid 224 and name C)	6.41	0.07	0.07
	assign	(segid 3A4 and resid 221 and name N)	(segid 3A4 and resid 224 and name CA)	5.60	0.06	0.06
	assign	(segid 3A4 and resid 221 and name N)	(segid 3A4 and resid 224 and name CB)	5.12	0.12	0.12
30	assign	(segid 3A4 and resid 221 and name N)	(segid 3A4 and resid 224 and name N)	4.78	0.04	0.05
	assign	(segid 3A4 and resid 221 and name N)	(segid 3A4 and resid 224 and name O)	7.59	0.07	0.08
	assign	(segid 3A4 and resid 221 and name N)	(segid 3A4 and resid 225 and name CA)	7.13	0.13	0.13
	assign	(segid 3A4 and resid 221 and name N)	(segid 3A4 and resid 225 and name CB)	6.88	0.17	0.17
	assign	(segid 3A4 and resid 221 and name N)	(segid 3A4 and resid 225 and name N)	6.04	0.10	0.10
35	assign	(segid 3A4 and resid 221 and name N)	(segid 3A4 and resid 248 and name CB)	7.04	0.37	0.37
	assign	(segid 3A4 and resid 221 and name O)	(segid 3A4 and resid 221 and name CB)	3.34	0.06	0.07
	assign	(segid 3A4 and resid 221 and name O)	(segid 3A4 and resid 222 and name C)	2.93	0.07	0.07
	assign	(segid 3A4 and resid 221 and name O)	(segid 3A4 and resid 222 and name CA)	2.77	0.06	0.06
	assign	(segid 3A4 and resid 221 and name O)	(segid 3A4 and resid 222 and name CB)	4.27	0.04	0.04
40	assign	(segid 3A4 and resid 221 and name O)	(segid 3A4 and resid 222 and name N)	2.25	0.02	0.01
	assign	(segid 3A4 and resid 221 and name O)	(segid 3A4 and resid 222 and name O)	3.43	0.07	0.06
	assign	(segid 3A4 and resid 221 and name O)	(segid 3A4 and resid 223 and name C)	3.99	0.13	0.12
	assign	(segid 3A4 and resid 221 and name O)	(segid 3A4 and resid 223 and name CA)	4.29	0.14	0.15
	assign	(segid 3A4 and resid 221 and name O)	(segid 3A4 and resid 223 and name CB)	5.25	0.17	0.16
45	assign	(segid 3A4 and resid 221 and name O)	(segid 3A4 and resid 223 and name N)	3.35	0.14	0.13
	assign	(segid 3A4 and resid 221 and name O)	(segid 3A4 and resid 223 and name O)	4.91	0.12	0.12
	assign	(segid 3A4 and resid 221 and name O)	(segid 3A4 and resid 224 and name C)	3.70	0.07	0.07
	assign	(segid 3A4 and resid 221 and name O)	(segid 3A4 and resid 224 and name CA)	3.68	0.12	0.12
	assign	(segid 3A4 and resid 221 and name O)	(segid 3A4 and resid 224 and name CB)	3.66	0.21	0.21
50	assign	(segid 3A4 and resid 221 and name O)	(segid 3A4 and resid 224 and name N)	3.19	0.14</	

	assign (segid 3A4 and resid 222 and name CA) (segid 3A4 and resid 223 and name C)	4.40	0.04	0.03
	assign (segid 3A4 and resid 222 and name CA) (segid 3A4 and resid 223 and name CA)	3.81	0.01	0.02
	assign (segid 3A4 and resid 222 and name CA) (segid 3A4 and resid 223 and name CB)	4.89	0.05	0.05
	assign (segid 3A4 and resid 222 and name CA) (segid 3A4 and resid 223 and name N)	2.44	0.02	0.02
5	assign (segid 3A4 and resid 222 and name CA) (segid 3A4 and resid 223 and name O)	5.29	0.09	0.10
	assign (segid 3A4 and resid 222 and name CA) (segid 3A4 and resid 224 and name C)	5.45	0.05	0.05
	assign (segid 3A4 and resid 222 and name CA) (segid 3A4 and resid 224 and name CA)	5.47	0.07	0.06
	assign (segid 3A4 and resid 222 and name CA) (segid 3A4 and resid 224 and name CB)	5.96	0.12	0.13
	assign (segid 3A4 and resid 222 and name CA) (segid 3A4 and resid 224 and name N)	4.39	0.07	0.07
10	assign (segid 3A4 and resid 222 and name CA) (segid 3A4 and resid 224 and name O)	6.55	0.07	0.07
	assign (segid 3A4 and resid 222 and name CA) (segid 3A4 and resid 225 and name C)	5.70	0.11	0.11
	assign (segid 3A4 and resid 222 and name CA) (segid 3A4 and resid 225 and name CA)	5.07	0.04	0.04
	assign (segid 3A4 and resid 222 and name CA) (segid 3A4 and resid 225 and name CB)	4.40	0.06	0.06
	assign (segid 3A4 and resid 222 and name CA) (segid 3A4 and resid 225 and name N)	4.54	0.08	0.08
15	assign (segid 3A4 and resid 222 and name CA) (segid 3A4 and resid 225 and name O)	6.86	0.11	0.11
	assign (segid 3A4 and resid 222 and name CA) (segid 3A4 and resid 226 and name C)	7.22	0.25	0.25
	assign (segid 3A4 and resid 222 and name CA) (segid 3A4 and resid 226 and name CA)	6.22	0.26	0.27
	assign (segid 3A4 and resid 222 and name CA) (segid 3A4 and resid 226 and name N)	5.23	0.21	0.20
	assign (segid 3A4 and resid 222 and name CA) (segid 3A4 and resid 240 and name CA)	13.52	0.51	0.52
20	assign (segid 3A4 and resid 222 and name CA) (segid 3A4 and resid 240 and name CB)	14.97	0.48	0.48
	assign (segid 3A4 and resid 222 and name CA) (segid 3A4 and resid 241 and name CA)	12.27	0.63	0.63
	assign (segid 3A4 and resid 222 and name CA) (segid 3A4 and resid 241 and name CB)	12.84	0.69	0.69
	assign (segid 3A4 and resid 222 and name CA) (segid 3A4 and resid 242 and name CA)	14.80	0.57	0.56
	assign (segid 3A4 and resid 222 and name CA) (segid 3A4 and resid 242 and name CB)	16.24	0.56	0.56
25	assign (segid 3A4 and resid 222 and name CA) (segid 3A4 and resid 243 and name CA)	13.85	0.40	0.39
	assign (segid 3A4 and resid 222 and name CA) (segid 3A4 and resid 243 and name CB)	13.98	0.39	0.38
	assign (segid 3A4 and resid 222 and name CA) (segid 3A4 and resid 244 and name CA)	10.22	0.42	0.43
	assign (segid 3A4 and resid 222 and name CA) (segid 3A4 and resid 244 and name CB)	9.26	0.49	0.49
	assign (segid 3A4 and resid 222 and name CA) (segid 3A4 and resid 245 and name CA)	12.02	0.43	0.43
30	assign (segid 3A4 and resid 222 and name CA) (segid 3A4 and resid 245 and name CB)	13.02	0.44	0.44
	assign (segid 3A4 and resid 222 and name CA) (segid 3A4 and resid 246 and name CA)	14.62	0.46	0.47
	assign (segid 3A4 and resid 222 and name CA) (segid 3A4 and resid 246 and name CB)	15.60	0.42	0.42
	assign (segid 3A4 and resid 222 and name CA) (segid 3A4 and resid 247 and name CA)	12.61	0.43	0.44
	assign (segid 3A4 and resid 222 and name CA) (segid 3A4 and resid 247 and name CB)	11.67	0.40	0.40
35	assign (segid 3A4 and resid 222 and name CA) (segid 3A4 and resid 248 and name CA)	11.01	0.60	0.60
	assign (segid 3A4 and resid 222 and name CA) (segid 3A4 and resid 248 and name CB)	10.22	0.67	0.67
	assign (segid 3A4 and resid 222 and name CA) (segid 3A4 and resid 249 and name CA)	14.62	0.66	0.67
	assign (segid 3A4 and resid 222 and name CA) (segid 3A4 and resid 250 and name CA)	16.04	0.62	0.62
	assign (segid 3A4 and resid 222 and name CA) (segid 3A4 and resid 250 and name CB)	16.12	0.60	0.59
40	assign (segid 3A4 and resid 222 and name CA) (segid 3A4 and resid 251 and name CA)	14.12	0.69	0.69
	assign (segid 3A4 and resid 222 and name CA) (segid 3A4 and resid 251 and name CB)	12.67	0.68	0.68
	assign (segid 3A4 and resid 222 and name CA) (segid 3A4 and resid 252 and name CA)	15.29	0.89	0.88
	assign (segid 3A4 and resid 222 and name CA) (segid 3A4 and resid 252 and name CB)	15.04	0.91	0.91
	assign (segid 3A4 and resid 222 and name CA) (segid 3A4 and resid 252 and name N)	18.32	0.39	0.39
45	assign (segid 3A4 and resid 222 and name CA) (segid 3A4 and resid 252 and name CB)	17.18	0.36	0.35
	assign (segid 3A4 and resid 222 and name CA) (segid 3A4 and resid 253 and name CA)	17.98	0.43	0.44
	assign (segid 3A4 and resid 222 and name CA) (segid 3A4 and resid 253 and name CB)	18.61	0.73	0.72
	assign (segid 3A4 and resid 222 and name CA) (segid 3A4 and resid 253 and name N)	17.25	0.67	0.68
	assign (segid 3A4 and resid 222 and name CB) (segid 3A4 and resid 223 and name C)	5.39	0.04	0.05
50	assign (segid 3A4 and resid 222 and name CB) (segid 3A4 and resid 223 and name CA)	4.45	0.06	0.06
	assign (segid 3A4 and resid 222 and name CB) (segid 3A4 and resid 223 and name CB)	5.34	0.10	0.11
	assign (segid 3A4 and resid 222 and name CB) (segid 3A4 and resid 223 and name N)	3.14	0.07	0.07
	assign (segid 3A4 and resid 222 and name CB) (segid 3A4 and resid 223 and name O)	6.24	0.09	0.10
	assign (segid 3A4 and resid 222 and name CB) (segid 3A4 and resid 224 and name C)	6.86	0.05	0.04
	assign (segid 3A4 and resid 222 and name CB) (segid 3A4 and resid 224 and name CA)	6.82	0.04	0.04
55	assign (segid 3A4 and resid 222 and name CB) (segid 3A4 and resid 224 and name CB)	7.38	0.08	0.08
	assign (segid 3A4 and resid 222 and name CB) (segid 3A4 and resid 224 and name N)	5.61	0.03	0.04
	assign (segid 3A4 and resid 222 and name CB) (segid 3A4 and resid 225 and name C)	6.86	0.15	0.15
	assign (segid 3A4 and resid 222 and name CB) (segid 3A4 and resid 225 and name CA)	6.42	0.08	0.08
	assign (segid 3A4 and resid 222 and name CB) (segid 3A4 and resid 225 and name CB)	5.66	0.08	0.08
60	assign (segid 3A4 and resid 222 and name CB) (segid 3A4 and resid 225 and name N)	5.97	0.10	0.10
	assign (segid 3A4 and resid 222 and name CB) (segid 3A4 and resid 226 and name CA)	7.00	0.29	0.30
	assign (segid 3A4 and resid 222 and name CB) (segid 3A4 and resid 226 and name N)	6.23	0.22	0.22
	assign (segid 3A4 and resid 222 and name CB) (segid 3A4 and resid 240 and name CA)	14.97	0.52	0.53
65	assign (segid 3A4 and resid 222 and name CB) (segid 3A4 and resid 240 and name CB)	16.43	0.49	0.49
	assign (segid 3A4 and resid 222 and name CB) (segid 3A4 and resid 241 and name CA)	13.70	0.64	0.63
	assign (segid 3A4 and resid 222 and name CB) (segid 3A4 and resid 241 and name CB)	14.20	0.70	0.71
	assign (segid 3A4 and resid 222 and name CB) (segid 3A4 and resid 242 and name CA)	16.26	0.57	0.58
	assign (segid 3A4 and resid 222 and name CB) (segid 3A4 and resid 242 and name CB)	17.71	0.57	0.57
70	assign (segid 3A4 and resid 222 and name CB) (segid 3A4 and resid 243 and name CA)	15.35	0.37	0.38
	assign (segid 3A4 and resid 222 and name CB) (segid 3A4 and resid 243 and name CB)	15.49	0.37	0.37
	assign (segid 3A4 and resid 222 and name CB) (segid 3A4 and resid 244 and name CA)	11.72	0.40	0.40
	assign (segid 3A4 and resid 222 and name CB) (segid 3A4 and resid 244 and name CB)	10.76	0.47	0.47
	assign (segid 3A4 and resid 222 and name CB) (segid 3A4 and resid 245 and name CA)	13.39	0.39	0.39
75	assign (segid 3A4 and resid 222 and name CB) (segid 3A4 and resid 245 and name CB)	14.38	0.42	0.41
	assign (segid 3A4 and resid 222 and name CB) (segid 3A4 and resid 246 and name CA)	16.01	0.40	0.40
	assign (segid 3A4 and resid 222 and name CB) (segid 3A4 and resid 246 and name CB)	17.03	0.37	0.36
	assign (segid 3A4 and resid 222 and name CB) (segid 3A4 and resid 247 and name CA)	13.94	0.34	0.34
	assign (segid 3A4 and resid 222 and name CB) (segid 3A4 and resid 247 and name CB)	13.02	0.33	0.32
80	assign (segid 3A4 and resid 222 and name CB) (segid 3A4 and resid 248 and name CA)	12.16	0.51	0.50
	assign (segid 3A4 and resid 222 and name CB) (segid 3A4 and resid 248 and name CB)	11.37	0.58	0.59
	assign (segid 3A4 and resid 222 and name CB) (segid 3A4 and resid 249 and name CA)	15.73	0.60	0.60
	assign (segid 3A4 and resid 222 and name CB) (segid 3A4 and resid 250 and name CA)	17.14	0.52	0.52

	assign (segid 3A4 and resid 222 and name CB)	(segid 3A4 and resid 250 and name CB)	17.28	0.51	0.51
	assign (segid 3A4 and resid 222 and name CB)	(segid 3A4 and resid 251 and name CA)	15.01	0.59	0.59
	assign (segid 3A4 and resid 222 and name CB)	(segid 3A4 and resid 251 and name CB)	13.54	0.58	0.58
	assign (segid 3A4 and resid 222 and name CB)	(segid 3A4 and resid 252 and name CA)	16.03	0.84	0.83
5	assign (segid 3A4 and resid 222 and name CB)	(segid 3A4 and resid 252 and name CB)	15.80	0.87	0.87
	assign (segid 3A4 and resid 222 and name CB)	(segid 3A4 and resid 392 and name CA)	19.01	0.40	0.40
	assign (segid 3A4 and resid 222 and name CB)	(segid 3A4 and resid 392 and name CB)	17.94	0.34	0.33
	assign (segid 3A4 and resid 222 and name CB)	(segid 3A4 and resid 393 and name CA)	18.47	0.43	0.43
	assign (segid 3A4 and resid 222 and name CB)	(segid 3A4 and resid 396 and name CA)	18.67	0.74	0.75
10	assign (segid 3A4 and resid 222 and name CB)	(segid 3A4 and resid 396 and name CB)	17.37	0.69	0.70
	assign (segid 3A4 and resid 222 and name N)	(segid 3A4 and resid 222 and name C)	2.44	0.03	0.03
	assign (segid 3A4 and resid 222 and name N)	(segid 3A4 and resid 222 and name CA)	1.46	0.01	0.01
	assign (segid 3A4 and resid 222 and name N)	(segid 3A4 and resid 222 and name CB)	2.47	0.04	0.04
	assign (segid 3A4 and resid 222 and name N)	(segid 3A4 and resid 222 and name O)	3.49	0.04	0.03
15	assign (segid 3A4 and resid 222 and name N)	(segid 3A4 and resid 223 and name C)	4.67	0.04	0.04
	assign (segid 3A4 and resid 222 and name N)	(segid 3A4 and resid 223 and name CA)	4.19	0.03	0.03
	assign (segid 3A4 and resid 222 and name N)	(segid 3A4 and resid 223 and name CB)	4.96	0.06	0.06
	assign (segid 3A4 and resid 222 and name N)	(segid 3A4 and resid 223 and name N)	2.79	0.03	0.03
	assign (segid 3A4 and resid 222 and name N)	(segid 3A4 and resid 223 and name O)	5.75	0.08	0.07
20	assign (segid 3A4 and resid 222 and name N)	(segid 3A4 and resid 224 and name C)	5.57	0.04	0.04
	assign (segid 3A4 and resid 222 and name N)	(segid 3A4 and resid 224 and name CA)	5.33	0.05	0.04
	assign (segid 3A4 and resid 222 and name N)	(segid 3A4 and resid 224 and name CB)	5.47	0.11	0.11
	assign (segid 3A4 and resid 222 and name N)	(segid 3A4 and resid 224 and name N)	4.30	0.06	0.07
	assign (segid 3A4 and resid 222 and name N)	(segid 3A4 and resid 224 and name O)	6.75	0.03	0.04
25	assign (segid 3A4 and resid 222 and name N)	(segid 3A4 and resid 225 and name C)	6.42	0.12	0.11
	assign (segid 3A4 and resid 222 and name N)	(segid 3A4 and resid 225 and name CA)	5.50	0.08	0.09
	assign (segid 3A4 and resid 222 and name N)	(segid 3A4 and resid 225 and name CB)	4.91	0.13	0.13
	assign (segid 3A4 and resid 222 and name N)	(segid 3A4 and resid 225 and name N)	4.76	0.06	0.07
	assign (segid 3A4 and resid 222 and name N)	(segid 3A4 and resid 225 and name O)	7.59	0.10	0.10
30	assign (segid 3A4 and resid 222 and name N)	(segid 3A4 and resid 226 and name CA)	7.27	0.24	0.23
	assign (segid 3A4 and resid 222 and name N)	(segid 3A4 and resid 226 and name N)	6.12	0.19	0.19
	assign (segid 3A4 and resid 222 and name O)	(segid 3A4 and resid 222 and name CB)	3.25	0.06	0.05
	assign (segid 3A4 and resid 222 and name O)	(segid 3A4 and resid 223 and name C)	3.00	0.04	0.05
35	assign (segid 3A4 and resid 222 and name O)	(segid 3A4 and resid 223 and name CA)	2.80	0.02	0.02
	assign (segid 3A4 and resid 222 and name O)	(segid 3A4 and resid 223 and name CB)	4.30	0.03	0.03
	assign (segid 3A4 and resid 222 and name O)	(segid 3A4 and resid 223 and name N)	2.27	0.02	0.01
	assign (segid 3A4 and resid 222 and name O)	(segid 3A4 and resid 223 and name O)	3.45	0.13	0.13
	assign (segid 3A4 and resid 222 and name O)	(segid 3A4 and resid 224 and name C)	4.13	0.06	0.07
	assign (segid 3A4 and resid 222 and name O)	(segid 3A4 and resid 224 and name CA)	4.43	0.09	0.10
40	assign (segid 3A4 and resid 222 and name O)	(segid 3A4 and resid 224 and name CB)	5.46	0.10	0.11
	assign (segid 3A4 and resid 222 and name O)	(segid 3A4 and resid 224 and name N)	3.49	0.08	0.08
	assign (segid 3A4 and resid 222 and name O)	(segid 3A4 and resid 224 and name O)	5.00	0.08	0.08
	assign (segid 3A4 and resid 222 and name O)	(segid 3A4 and resid 225 and name C)	3.96	0.09	0.09
45	assign (segid 3A4 and resid 222 and name O)	(segid 3A4 and resid 225 and name CA)	3.85	0.16	0.16
	assign (segid 3A4 and resid 222 and name O)	(segid 3A4 and resid 225 and name CB)	3.71	0.20	0.21
	assign (segid 3A4 and resid 222 and name O)	(segid 3A4 and resid 225 and name N)	3.39	0.21	0.20
	assign (segid 3A4 and resid 222 and name O)	(segid 3A4 and resid 225 and name O)	5.12	0.10	0.09
	assign (segid 3A4 and resid 222 and name O)	(segid 3A4 and resid 226 and name C)	4.88	0.24	0.24
50	assign (segid 3A4 and resid 222 and name O)	(segid 3A4 and resid 226 and name CA)	3.97	0.23	0.23
	assign (segid 3A4 and resid 222 and name O)	(segid 3A4 and resid 226 and name N)	3.14	0.15	0.15
	assign (segid 3A4 and resid 222 and name O)	(segid 3A4 and resid 226 and name O)	5.76	0.32	0.33
	assign (segid 3A4 and resid 223 and name C)	(segid 3A4 and resid 223 and name CB)	2.49	0.02	0.02
	assign (segid 3A4 and resid 223 and name C)	(segid 3A4 and resid 223 and name O)	1.23	0.00	0.00
55	assign (segid 3A4 and resid 223 and name C)	(segid 3A4 and resid 224 and name C)	3.05	0.05	0.06
	assign (segid 3A4 and resid 223 and name C)	(segid 3A4 and resid 224 and name CA)	2.43	0.01	0.02
	assign (segid 3A4 and resid 223 and name C)	(segid 3A4 and resid 224 and name CB)	3.70	0.02	0.03
	assign (segid 3A4 and resid 223 and name C)	(segid 3A4 and resid 224 and name N)	1.33	0.01	0.00
	assign (segid 3A4 and resid 223 and name C)	(segid 3A4 and resid 224 and name O)	3.88	0.17	0.17
60	assign (segid 3A4 and resid 223 and name C)	(segid 3A4 and resid 225 and name C)	4.75	0.09	0.10
	assign (segid 3A4 and resid 223 and name C)	(segid 3A4 and resid 225 and name CA)	4.57	0.09	0.09
	assign (segid 3A4 and resid 223 and name C)	(segid 3A4 and resid 225 and name CB)	5.28	0.13	0.13
	assign (segid 3A4 and resid 223 and name C)	(segid 3A4 and resid 225 and name N)	3.36	0.11	0.10
	assign (segid 3A4 and resid 223 and name C)	(segid 3A4 and resid 225 and name O)	5.85	0.12	0.12
	assign (segid 3A4 and resid 223 and name C)	(segid 3A4 and resid 226 and name C)	4.84	0.08	0.07
65	assign (segid 3A4 and resid 223 and name C)	(segid 3A4 and resid 226 and name CA)	4.81	0.07	0.08
	assign (segid 3A4 and resid 223 and name C)	(segid 3A4 and resid 226 and name N)	4.04	0.08	0.08
	assign (segid 3A4 and resid 223 and name C)	(segid 3A4 and resid 226 and name O)	5.69	0.35	0.35
	assign (segid 3A4 and resid 223 and name CA)	(segid 3A4 and resid 223 and name C)	1.52	0.01	0.01
70	assign (segid 3A4 and resid 223 and name CA)	(segid 3A4 and resid 223 and name CB)	1.54	0.02	0.01
	assign (segid 3A4 and resid 223 and name CA)	(segid 3A4 and resid 223 and name O)	2.38	0.02	0.01
	assign (segid 3A4 and resid 223 and name CA)	(segid 3A4 and resid 224 and name C)	4.43	0.05	0.06
	assign (segid 3A4 and resid 223 and name CA)	(segid 3A4 and resid 224 and name CA)	3.81	0.01	0.01
	assign (segid 3A4 and resid 223 and name CA)	(segid 3A4 and resid 224 and name CB)	4.87	0.02	0.03
	assign (segid 3A4 and resid 223 and name CA)	(segid 3A4 and resid 224 and name N)	2.44	0.03	0.03
75	assign (segid 3A4 and resid 223 and name CA)	(segid 3A4 and resid 224 and name O)	5.33	0.17	0.17
	assign (segid 3A4 and resid 223 and name CA)	(segid 3A4 and resid 225 and name C)	5.71	0.09	0.08
	assign (segid 3A4 and resid 223 and name CA)	(segid 3A4 and resid 225 and name CA)	5.55	0.10	0.10
	assign (segid 3A4 and resid 223 and name CA)	(segid 3A4 and resid 225 and name CB)	5.92	0.14	0.15
	assign (segid 3A4 and resid 223 and name CA)	(segid 3A4 and resid 225 and name N)	4.45	0.11	0.10
80	assign (segid 3A4 and resid 223 and name CA)	(segid 3A4 and resid 225 and name O)	6.85	0.08	0.08
	assign (segid 3A4 and resid 223 and name CA)	(segid 3A4 and resid 226 and name C)	5.64	0.08	0.09
	assign (segid 3A4 and resid 223 and name CA)	(segid 3A4 and resid 226 and name CA)	5.45	0.08	0.09
	assign (segid 3A4 and resid 223 and name CA)	(segid 3A4 and resid 226 and name N)	4.82	0.08	0.08

	assign (segid 3A4 and resid 223 and name CA)	(segid 3A4 and resid 226 and name O)	6.38	0.35	0.34
	assign (segid 3A4 and resid 223 and name CA)	(segid 3A4 and resid 240 and name CA)	13.31	0.48	0.48
	assign (segid 3A4 and resid 223 and name CA)	(segid 3A4 and resid 210 and name CB)	14.73	0.44	0.43
	assign (segid 3A4 and resid 223 and name CA)	(segid 3A4 and resid 241 and name CB)	13.05	0.52	0.53
5	assign (segid 3A4 and resid 223 and name CA)	(segid 3A4 and resid 241 and name CB)	13.95	0.57	0.58
	assign (segid 3A4 and resid 223 and name CA)	(segid 3A4 and resid 242 and name CA)	15.31	0.43	0.42
	assign (segid 3A4 and resid 223 and name CA)	(segid 3A4 and resid 242 and name CB)	16.65	0.40	0.41
	assign (segid 3A4 and resid 223 and name CA)	(segid 3A4 and resid 243 and name CA)	13.47	0.32	0.33
	assign (segid 3A4 and resid 223 and name CA)	(segid 3A4 and resid 243 and name CB)	13.25	0.32	0.33
10	assign (segid 3A4 and resid 223 and name CA)	(segid 3A4 and resid 244 and name CA)	10.27	0.35	0.35
	assign (segid 3A4 and resid 223 and name CA)	(segid 3A4 and resid 244 and name CB)	9.61	0.42	0.43
	assign (segid 3A4 and resid 223 and name CA)	(segid 3A4 and resid 245 and name CA)	12.89	0.32	0.32
	assign (segid 3A4 and resid 223 and name CA)	(segid 3A4 and resid 245 and name CB)	14.11	0.33	0.33
	assign (segid 3A4 and resid 223 and name CA)	(segid 3A4 and resid 246 and name CA)	14.72	0.40	0.40
	assign (segid 3A4 and resid 223 and name CA)	(segid 3A4 and resid 246 and name CB)	15.48	0.38	0.39
15	assign (segid 3A4 and resid 223 and name CA)	(segid 3A4 and resid 247 and name CA)	12.06	0.45	0.46
	assign (segid 3A4 and resid 223 and name CA)	(segid 3A4 and resid 247 and name CB)	10.83	0.46	0.47
	assign (segid 3A4 and resid 223 and name CA)	(segid 3A4 and resid 248 and name CA)	11.41	0.50	0.51
	assign (segid 3A4 and resid 223 and name CA)	(segid 3A4 and resid 248 and name CB)	11.08	0.58	0.58
20	assign (segid 3A4 and resid 223 and name CA)	(segid 3A4 and resid 249 and name CA)	15.19	0.50	0.50
	assign (segid 3A4 and resid 223 and name CA)	(segid 3A4 and resid 250 and name CA)	15.74	0.56	0.55
	assign (segid 3A4 and resid 223 and name CA)	(segid 3A4 and resid 250 and name CB)	15.52	0.65	0.64
	assign (segid 3A4 and resid 223 and name CA)	(segid 3A4 and resid 251 and name CA)	13.72	0.58	0.59
	assign (segid 3A4 and resid 223 and name CA)	(segid 3A4 and resid 251 and name CB)	12.25	0.60	0.60
25	assign (segid 3A4 and resid 223 and name CA)	(segid 3A4 and resid 252 and name CA)	15.74	0.67	0.68
	assign (segid 3A4 and resid 223 and name CA)	(segid 3A4 and resid 252 and name CB)	15.82	0.70	0.70
	assign (segid 3A4 and resid 223 and name CA)	(segid 3A4 and resid 392 and name CA)	16.00	0.55	0.56
	assign (segid 3A4 and resid 223 and name CA)	(segid 3A4 and resid 392 and name CB)	14.87	0.53	0.54
	assign (segid 3A4 and resid 223 and name CA)	(segid 3A4 and resid 393 and name CA)	16.20	0.57	0.56
30	assign (segid 3A4 and resid 223 and name CA)	(segid 3A4 and resid 395 and name CA)	18.61	0.74	0.75
	assign (segid 3A4 and resid 223 and name CA)	(segid 3A4 and resid 396 and name CA)	17.18	0.80	0.79
	assign (segid 3A4 and resid 223 and name CA)	(segid 3A4 and resid 396 and name CB)	15.93	0.76	0.75
	assign (segid 3A4 and resid 223 and name CB)	(segid 3A4 and resid 224 and name C)	5.44	0.06	0.06
	assign (segid 3A4 and resid 223 and name CB)	(segid 3A4 and resid 224 and name CA)	4.46	0.06	0.05
	assign (segid 3A4 and resid 223 and name CB)	(segid 3A4 and resid 224 and name CB)	5.30	0.09	0.08
35	assign (segid 3A4 and resid 223 and name CB)	(segid 3A4 and resid 224 and name N)	3.14	0.07	0.08
	assign (segid 3A4 and resid 223 and name CB)	(segid 3A4 and resid 224 and name O)	6.30	0.17	0.16
	assign (segid 3A4 and resid 223 and name CB)	(segid 3A4 and resid 225 and name C)	7.11	0.09	0.09
	assign (segid 3A4 and resid 223 and name CB)	(segid 3A4 and resid 225 and name CA)	6.89	0.09	0.09
	assign (segid 3A4 and resid 223 and name CB)	(segid 3A4 and resid 225 and name CB)	7.33	0.15	0.14
40	assign (segid 3A4 and resid 223 and name CB)	(segid 3A4 and resid 225 and name N)	5.66	0.09	0.09
	assign (segid 3A4 and resid 223 and name CB)	(segid 3A4 and resid 226 and name C)	6.82	0.09	0.09
	assign (segid 3A4 and resid 223 and name CB)	(segid 3A4 and resid 226 and name CA)	6.83	0.08	0.08
	assign (segid 3A4 and resid 223 and name CB)	(segid 3A4 and resid 226 and name N)	6.26	0.09	0.09
	assign (segid 3A4 and resid 223 and name CB)	(segid 3A4 and resid 226 and name O)	7.46	0.39	0.38
45	assign (segid 3A4 and resid 223 and name CB)	(segid 3A4 and resid 240 and name CA)	14.19	0.51	0.50
	assign (segid 3A4 and resid 223 and name CB)	(segid 3A4 and resid 240 and name CB)	15.55	0.48	0.48
	assign (segid 3A4 and resid 223 and name CB)	(segid 3A4 and resid 241 and name CA)	14.01	0.53	0.53
	assign (segid 3A4 and resid 223 and name CB)	(segid 3A4 and resid 241 and name CB)	14.99	0.58	0.59
50	assign (segid 3A4 and resid 223 and name CB)	(segid 3A4 and resid 242 and name CA)	15.99	0.44	0.45
	assign (segid 3A4 and resid 223 and name CB)	(segid 3A4 and resid 242 and name CB)	17.34	0.41	0.41
	assign (segid 3A4 and resid 223 and name CB)	(segid 3A4 and resid 243 and name CA)	13.91	0.35	0.34
	assign (segid 3A4 and resid 223 and name CB)	(segid 3A4 and resid 243 and name CB)	13.68	0.33	0.34
	assign (segid 3A4 and resid 223 and name CB)	(segid 3A4 and resid 244 and name CA)	10.79	0.36	0.35
55	assign (segid 3A4 and resid 223 and name CB)	(segid 3A4 and resid 244 and name CB)	10.31	0.40	0.41
	assign (segid 3A4 and resid 223 and name CB)	(segid 3A4 and resid 245 and name CA)	13.35	0.33	0.33
	assign (segid 3A4 and resid 223 and name CB)	(segid 3A4 and resid 245 and name CB)	14.65	0.33	0.33
	assign (segid 3A4 and resid 223 and name CB)	(segid 3A4 and resid 246 and name CA)	14.86	0.39	0.39
	assign (segid 3A4 and resid 223 and name CB)	(segid 3A4 and resid 246 and name CB)	15.63	0.42	0.43
60	assign (segid 3A4 and resid 223 and name CB)	(segid 3A4 and resid 247 and name CA)	11.92	0.46	0.46
	assign (segid 3A4 and resid 223 and name CB)	(segid 3A4 and resid 247 and name CB)	10.70	0.49	0.48
	assign (segid 3A4 and resid 223 and name CB)	(segid 3A4 and resid 248 and name CA)	11.33	0.42	0.42
	assign (segid 3A4 and resid 223 and name CB)	(segid 3A4 and resid 248 and name CB)	11.16	0.49	0.50
	assign (segid 3A4 and resid 223 and name CB)	(segid 3A4 and resid 249 and name CA)	15.07	0.42	0.42
65	assign (segid 3A4 and resid 223 and name CB)	(segid 3A4 and resid 250 and name CA)	15.31	0.52	0.53
	assign (segid 3A4 and resid 223 and name CB)	(segid 3A4 and resid 250 and name CB)	15.08	0.67	0.67
	assign (segid 3A4 and resid 223 and name CB)	(segid 3A4 and resid 251 and name CA)	13.07	0.50	0.50
	assign (segid 3A4 and resid 223 and name CB)	(segid 3A4 and resid 251 and name CB)	11.59	0.52	0.52
	assign (segid 3A4 and resid 223 and name CB)	(segid 3A4 and resid 252 and name CA)	15.23	0.57	0.57
70	assign (segid 3A4 and resid 223 and name CB)	(segid 3A4 and resid 252 and name CB)	15.44	0.59	0.59
	assign (segid 3A4 and resid 223 and name CB)	(segid 3A4 and resid 253 and name CA)	18.44	0.49	0.49
	assign (segid 3A4 and resid 223 and name CB)	(segid 3A4 and resid 254 and name CA)	18.10	0.73	0.72
	assign (segid 3A4 and resid 223 and name CB)	(segid 3A4 and resid 255 and name CA)	17.21	1.10	1.10
	assign (segid 3A4 and resid 223 and name CB)	(segid 3A4 and resid 391 and name CA)	18.37	0.65	0.65
75	assign (segid 3A4 and resid 223 and name CB)	(segid 3A4 and resid 392 and name CA)	14.77	0.63	0.63
	assign (segid 3A4 and resid 223 and name CB)	(segid 3A4 and resid 392 and name CB)	13.70	0.60	0.60
	assign (segid 3A4 and resid 223 and name CB)	(segid 3A4 and resid 393 and name CA)	14.91	0.61	0.61
	assign (segid 3A4 and resid 223 and name CB)	(segid 3A4 and resid 394 and name CA)	18.14	0.66	0.67
	assign (segid 3A4 and resid 223 and name CB)	(segid 3A4 and resid 394 and name CB)	18.87	0.69	0.68
80	assign (segid 3A4 and resid 223 and name CB)	(segid 3A4 and resid 395 and name CA)	17.15	0.76	0.77
	assign (segid 3A4 and resid 223 and name CB)	(segid 3A4 and resid 396 and name CA)	15.80	0.81	0.81
	assign (segid 3A4 and resid 223 and name CB)	(segid 3A4 and resid 396 and name CB)	14.58	0.78	0.77
	assign (segid 3A4 and resid 223 and name CB)	(segid 3A4 and resid 397 and name CA)	18.90	0.72	0.72

	assign (segid 3A4 and resid 223 and name CB)	(segid 3A4 and resid 399 and name CB)	18.76	0.85	0.85
	assign (segid 3A4 and resid 223 and name N)	(segid 3A4 and resid 223 and name C)	2.43	0.03	0.03
	assign (segid 3A4 and resid 223 and name N)	(segid 3A4 and resid 223 and name CA)	1.46	0.01	0.01
	assign (segid 3A4 and resid 223 and name N)	(segid 3A4 and resid 223 and name CB)	2.48	0.03	0.03
5	assign (segid 3A4 and resid 223 and name N)	(segid 3A4 and resid 223 and name O)	3.46	0.05	0.05
	assign (segid 3A4 and resid 223 and name N)	(segid 3A4 and resid 224 and name C)	4.68	0.05	0.04
	assign (segid 3A4 and resid 223 and name N)	(segid 3A4 and resid 224 and name CA)	4.20	0.04	0.03
	assign (segid 3A4 and resid 223 and name N)	(segid 3A4 and resid 224 and name CB)	4.99	0.07	0.07
	assign (segid 3A4 and resid 223 and name N)	(segid 3A4 and resid 224 and name N)	2.80	0.04	0.04
10	assign (segid 3A4 and resid 223 and name N)	(segid 3A4 and resid 224 and name O)	5.74	0.13	0.13
	assign (segid 3A4 and resid 223 and name N)	(segid 3A4 and resid 225 and name C)	5.73	0.05	0.06
	assign (segid 3A4 and resid 223 and name N)	(segid 3A4 and resid 225 and name CA)	5.33	0.05	0.05
	assign (segid 3A4 and resid 223 and name N)	(segid 3A4 and resid 225 and name CB)	5.35	0.12	0.12
	assign (segid 3A4 and resid 223 and name N)	(segid 3A4 and resid 225 and name N)	4.32	0.06	0.06
15	assign (segid 3A4 and resid 223 and name N)	(segid 3A4 and resid 225 and name O)	6.94	0.05	0.06
	assign (segid 3A4 and resid 223 and name N)	(segid 3A4 and resid 226 and name C)	6.35	0.15	0.14
	assign (segid 3A4 and resid 223 and name N)	(segid 3A4 and resid 226 and name CA)	5.82	0.15	0.15
	assign (segid 3A4 and resid 223 and name N)	(segid 3A4 and resid 226 and name N)	4.98	0.09	0.09
	assign (segid 3A4 and resid 223 and name N)	(segid 3A4 and resid 226 and name O)	7.17	0.32	0.33
20	assign (segid 3A4 and resid 223 and name N)	(segid 3A4 and resid 226 and name CB)	3.27	0.09	0.08
	assign (segid 3A4 and resid 223 and name O)	(segid 3A4 and resid 224 and name C)	3.05	0.06	0.06
	assign (segid 3A4 and resid 223 and name O)	(segid 3A4 and resid 224 and name CA)	2.76	0.04	0.04
	assign (segid 3A4 and resid 223 and name O)	(segid 3A4 and resid 224 and name CB)	4.23	0.06	0.06
	assign (segid 3A4 and resid 223 and name O)	(segid 3A4 and resid 224 and name N)	2.24	0.01	0.02
25	assign (segid 3A4 and resid 223 and name O)	(segid 3A4 and resid 224 and name O)	3.51	0.21	0.22
	assign (segid 3A4 and resid 223 and name O)	(segid 3A4 and resid 225 and name C)	4.41	0.16	0.16
	assign (segid 3A4 and resid 223 and name O)	(segid 3A4 and resid 225 and name CA)	4.58	0.15	0.15
	assign (segid 3A4 and resid 223 and name O)	(segid 3A4 and resid 225 and name CB)	5.50	0.19	0.19
	assign (segid 3A4 and resid 223 and name O)	(segid 3A4 and resid 225 and name N)	3.56	0.15	0.15
30	assign (segid 3A4 and resid 223 and name O)	(segid 3A4 and resid 225 and name O)	5.37	0.22	0.21
	assign (segid 3A4 and resid 223 and name O)	(segid 3A4 and resid 226 and name C)	3.84	0.11	0.11
	assign (segid 3A4 and resid 223 and name O)	(segid 3A4 and resid 226 and name CA)	4.10	0.15	0.16
	assign (segid 3A4 and resid 223 and name O)	(segid 3A4 and resid 226 and name N)	3.60	0.16	0.15
	assign (segid 3A4 and resid 223 and name O)	(segid 3A4 and resid 226 and name O)	4.62	0.38	0.38
35	assign (segid 3A4 and resid 223 and name O)	(segid 3A4 and resid 226 and name CB)	2.49	0.05	0.04
	assign (segid 3A4 and resid 224 and name C)	(segid 3A4 and resid 224 and name O)	1.23	0.01	0.01
	assign (segid 3A4 and resid 224 and name C)	(segid 3A4 and resid 225 and name C)	3.06	0.08	0.07
	assign (segid 3A4 and resid 224 and name C)	(segid 3A4 and resid 225 and name CA)	2.45	0.01	0.01
	assign (segid 3A4 and resid 224 and name C)	(segid 3A4 and resid 225 and name CB)	3.71	0.03	0.04
40	assign (segid 3A4 and resid 224 and name C)	(segid 3A4 and resid 225 and name N)	1.32	0.01	0.02
	assign (segid 3A4 and resid 224 and name C)	(segid 3A4 and resid 225 and name O)	3.92	0.16	0.16
	assign (segid 3A4 and resid 224 and name C)	(segid 3A4 and resid 226 and name C)	4.58	0.17	0.17
	assign (segid 3A4 and resid 224 and name C)	(segid 3A4 and resid 226 and name CA)	4.47	0.11	0.11
	assign (segid 3A4 and resid 224 and name C)	(segid 3A4 and resid 226 and name N)	3.28	0.10	0.10
45	assign (segid 3A4 and resid 224 and name C)	(segid 3A4 and resid 226 and name O)	5.67	0.29	0.30
	assign (segid 3A4 and resid 224 and name C)	(segid 3A4 and resid 244 and name CA)	6.64	0.62	0.62
	assign (segid 3A4 and resid 224 and name C)	(segid 3A4 and resid 244 and name CB)	5.83	0.61	0.61
	assign (segid 3A4 and resid 224 and name CA)	(segid 3A4 and resid 224 and name C)	1.53	0.01	0.01
50	assign (segid 3A4 and resid 224 and name CA)	(segid 3A4 and resid 224 and name CB)	1.52	0.02	0.02
	assign (segid 3A4 and resid 224 and name CA)	(segid 3A4 and resid 224 and name O)	2.39	0.02	0.01
	assign (segid 3A4 and resid 224 and name CA)	(segid 3A4 and resid 225 and name C)	4.47	0.06	0.06
	assign (segid 3A4 and resid 224 and name CA)	(segid 3A4 and resid 225 and name CA)	3.83	0.02	0.02
	assign (segid 3A4 and resid 224 and name CA)	(segid 3A4 and resid 225 and name CB)	4.87	0.04	0.04
	assign (segid 3A4 and resid 224 and name CA)	(segid 3A4 and resid 225 and name N)	2.44	0.02	0.03
55	assign (segid 3A4 and resid 224 and name CA)	(segid 3A4 and resid 225 and name O)	5.39	0.16	0.16
	assign (segid 3A4 and resid 224 and name CA)	(segid 3A4 and resid 226 and name C)	5.47	0.14	0.13
	assign (segid 3A4 and resid 224 and name CA)	(segid 3A4 and resid 226 and name CA)	5.52	0.06	0.07
	assign (segid 3A4 and resid 224 and name CA)	(segid 3A4 and resid 226 and name N)	4.43	0.05	0.05
	assign (segid 3A4 and resid 224 and name CA)	(segid 3A4 and resid 226 and name O)	6.47	0.30	0.30
60	assign (segid 3A4 and resid 224 and name CA)	(segid 3A4 and resid 240 and name CA)	9.86	0.52	0.52
	assign (segid 3A4 and resid 224 and name CA)	(segid 3A4 and resid 240 and name CB)	11.21	0.48	0.48
	assign (segid 3A4 and resid 224 and name CA)	(segid 3A4 and resid 241 and name CA)	9.79	0.53	0.53
	assign (segid 3A4 and resid 224 and name CA)	(segid 3A4 and resid 241 and name CB)	10.87	0.61	0.61
	assign (segid 3A4 and resid 224 and name CA)	(segid 3A4 and resid 242 and name CA)	11.77	0.39	0.39
65	assign (segid 3A4 and resid 224 and name CA)	(segid 3A4 and resid 242 and name CB)	13.08	0.37	0.36
	assign (segid 3A4 and resid 224 and name CA)	(segid 3A4 and resid 243 and name CA)	9.77	0.32	0.33
	assign (segid 3A4 and resid 224 and name CA)	(segid 3A4 and resid 243 and name CB)	9.53	0.29	0.29
	assign (segid 3A4 and resid 224 and name CA)	(segid 3A4 and resid 244 and name CA)	6.77	0.39	0.39
	assign (segid 3A4 and resid 224 and name CA)	(segid 3A4 and resid 244 and name CB)	6.23	0.42	0.42
70	assign (segid 3A4 and resid 224 and name CA)	(segid 3A4 and resid 245 and name CA)	9.83	0.41	0.41
	assign (segid 3A4 and resid 224 and name CA)	(segid 3A4 and resid 245 and name CB)	11.04	0.39	0.38
	assign (segid 3A4 and resid 224 and name CA)	(segid 3A4 and resid 246 and name CA)	11.47	0.55	0.55
	assign (segid 3A4 and resid 224 and name CA)	(segid 3A4 and resid 246 and name CB)	12.08	0.49	0.48
	assign (segid 3A4 and resid 224 and name CA)	(segid 3A4 and resid 247 and name CA)	9.09	0.67	0.68
75	assign (segid 3A4 and resid 224 and name CA)	(segid 3A4 and resid 247 and name CB)	7.78	0.65	0.66
	assign (segid 3A4 and resid 224 and name CA)	(segid 3A4 and resid 248 and name CA)	9.17	0.80	0.79
	assign (segid 3A4 and resid 224 and name CA)	(segid 3A4 and resid 248 and name CB)	8.90	0.81	0.80
	assign (segid 3A4 and resid 224 and name CA)	(segid 3A4 and resid 249 and name CA)	12.83	0.74	0.74
	assign (segid 3A4 and resid 224 and name CA)	(segid 3A4 and resid 250 and name CA)	13.40	0.80	0.80
80	assign (segid 3A4 and resid 224 and name CA)	(segid 3A4 and resid 250 and name CB)	13.01	0.82	0.82
	assign (segid 3A4 and resid 224 and name CA)	(segid 3A4 and resid 251 and name CA)	12.18	0.91	0.91
	assign (segid 3A4 and resid 224 and name CA)	(segid 3A4 and resid 251 and name CB)	10.85	0.96	0.95
	assign (segid 3A4 and resid 224 and name CA)	(segid 3A4 and resid 252 and name CA)	14.46	0.94	0.94

	assign (segid 3A4 and resid 224 and name CA)	(segid 3A4 and resid 252 and name CB)	14.44	0.94	0.93
	assign (segid 3A4 and resid 224 and name CA)	(segid 3A4 and resid 253 and name CA)	17.31	0.83	0.84
	assign (segid 3A4 and resid 224 and name CA)	(segid 3A4 and resid 254 and name CA)	17.36	1.00	1.00
	assign (segid 3A4 and resid 224 and name CA)	(segid 3A4 and resid 255 and name CA)	17.30	1.35	1.34
5	assign (segid 3A4 and resid 224 and name CA)	(segid 3A4 and resid 391 and name CA)	18.50	0.71	0.72
	assign (segid 3A4 and resid 224 and name CA)	(segid 3A4 and resid 392 and name CA)	15.23	0.58	0.57
	assign (segid 3A4 and resid 224 and name CA)	(segid 3A4 and resid 392 and name CB)	13.88	0.60	0.59
	assign (segid 3A4 and resid 224 and name CA)	(segid 3A4 and resid 393 and name CA)	15.92	0.65	0.65
	assign (segid 3A4 and resid 224 and name CA)	(segid 3A4 and resid 396 and name CA)	17.96	0.71	0.72
10	assign (segid 3A4 and resid 224 and name CA)	(segid 3A4 and resid 396 and name CB)	16.61	0.71	0.72
	assign (segid 3A4 and resid 224 and name CB)	(segid 3A4 and resid 225 and name C)	5.44	0.11	0.11
	assign (segid 3A4 and resid 224 and name CB)	(segid 3A4 and resid 225 and name CB)	4.47	0.11	0.11
	assign (segid 3A4 and resid 224 and name CB)	(segid 3A4 and resid 225 and name CB)	5.35	0.15	0.15
	assign (segid 3A4 and resid 224 and name CB)	(segid 3A4 and resid 225 and name N)	3.16	0.14	0.13
15	assign (segid 3A4 and resid 224 and name CB)	(segid 3A4 and resid 225 and name O)	6.30	0.18	0.19
	assign (segid 3A4 and resid 224 and name CB)	(segid 3A4 and resid 226 and name C)	6.88	0.15	0.14
	assign (segid 3A4 and resid 224 and name CB)	(segid 3A4 and resid 226 and name CA)	6.85	0.09	0.09
	assign (segid 3A4 and resid 224 and name CB)	(segid 3A4 and resid 226 and name N)	5.64	0.08	0.08
	assign (segid 3A4 and resid 224 and name CB)	(segid 3A4 and resid 240 and name CA)	9.57	0.70	0.69
20	assign (segid 3A4 and resid 224 and name CB)	(segid 3A4 and resid 240 and name CB)	10.84	0.63	0.64
	assign (segid 3A4 and resid 224 and name CB)	(segid 3A4 and resid 241 and name CA)	9.20	0.72	0.72
	assign (segid 3A4 and resid 224 and name CB)	(segid 3A4 and resid 241 and name CB)	10.33	0.80	0.80
	assign (segid 3A4 and resid 224 and name CB)	(segid 3A4 and resid 242 and name CA)	10.85	0.49	0.48
	assign (segid 3A4 and resid 224 and name CB)	(segid 3A4 and resid 242 and name CB)	12.19	0.45	0.44
25	assign (segid 3A4 and resid 224 and name CB)	(segid 3A4 and resid 243 and name CA)	8.83	0.31	0.30
	assign (segid 3A4 and resid 224 and name CB)	(segid 3A4 and resid 243 and name CB)	8.75	0.27	0.27
	assign (segid 3A4 and resid 224 and name CB)	(segid 3A4 and resid 244 and name C)	6.41	0.38	0.38
	assign (segid 3A4 and resid 224 and name CB)	(segid 3A4 and resid 244 and name CA)	5.68	0.37	0.37
	assign (segid 3A4 and resid 224 and name CB)	(segid 3A4 and resid 244 and name CB)	5.30	0.46	0.47
30	assign (segid 3A4 and resid 224 and name CB)	(segid 3A4 and resid 244 and name N)	6.79	0.35	0.36
	assign (segid 3A4 and resid 224 and name CB)	(segid 3A4 and resid 244 and name O)	6.18	0.52	0.52
	assign (segid 3A4 and resid 224 and name CB)	(segid 3A4 and resid 245 and name CA)	8.55	0.35	0.36
	assign (segid 3A4 and resid 224 and name CB)	(segid 3A4 and resid 245 and name CB)	9.83	0.35	0.34
	assign (segid 3A4 and resid 224 and name CB)	(segid 3A4 and resid 246 and name CA)	10.12	0.50	0.49
35	assign (segid 3A4 and resid 224 and name CB)	(segid 3A4 and resid 246 and name CB)	10.79	0.44	0.44
	assign (segid 3A4 and resid 224 and name CB)	(segid 3A4 and resid 247 and name CA)	7.72	0.69	0.69
	assign (segid 3A4 and resid 224 and name CB)	(segid 3A4 and resid 247 and name CB)	6.47	0.66	0.67
	assign (segid 3A4 and resid 224 and name CB)	(segid 3A4 and resid 248 and name CA)	7.73	0.82	0.82
	assign (segid 3A4 and resid 224 and name CB)	(segid 3A4 and resid 248 and name CB)	7.50	0.78	0.79
40	assign (segid 3A4 and resid 224 and name CB)	(segid 3A4 and resid 249 and name CA)	11.37	0.75	0.75
	assign (segid 3A4 and resid 224 and name CB)	(segid 3A4 and resid 250 and name CA)	11.99	0.87	0.86
	assign (segid 3A4 and resid 224 and name CB)	(segid 3A4 and resid 250 and name CB)	11.63	0.87	0.88
	assign (segid 3A4 and resid 224 and name CB)	(segid 3A4 and resid 251 and name CA)	10.88	1.02	1.02
	assign (segid 3A4 and resid 224 and name CB)	(segid 3A4 and resid 251 and name CB)	9.59	1.08	1.07
45	assign (segid 3A4 and resid 224 and name CB)	(segid 3A4 and resid 252 and name CA)	13.13	1.02	1.01
	assign (segid 3A4 and resid 224 and name CB)	(segid 3A4 and resid 252 and name CB)	13.08	0.99	0.98
	assign (segid 3A4 and resid 224 and name CB)	(segid 3A4 and resid 253 and name CA)	15.92	0.91	0.90
	assign (segid 3A4 and resid 224 and name CB)	(segid 3A4 and resid 254 and name CA)	16.07	1.10	1.10
	assign (segid 3A4 and resid 224 and name CB)	(segid 3A4 and resid 255 and name CA)	16.12	1.43	1.43
50	assign (segid 3A4 and resid 224 and name CB)	(segid 3A4 and resid 256 and name CA)	18.45	0.89	0.88
	assign (segid 3A4 and resid 224 and name CB)	(segid 3A4 and resid 391 and name CA)	17.71	0.84	0.83
	assign (segid 3A4 and resid 224 and name CB)	(segid 3A4 and resid 391 and name CB)	18.51	0.80	0.80
	assign (segid 3A4 and resid 224 and name CB)	(segid 3A4 and resid 392 and name CA)	14.57	0.68	0.67
	assign (segid 3A4 and resid 224 and name CB)	(segid 3A4 and resid 392 and name CB)	13.19	0.69	0.68
55	assign (segid 3A4 and resid 224 and name CB)	(segid 3A4 and resid 393 and name CA)	15.18	0.76	0.76
	assign (segid 3A4 and resid 224 and name CB)	(segid 3A4 and resid 396 and name CA)	17.42	0.76	0.77
	assign (segid 3A4 and resid 224 and name CB)	(segid 3A4 and resid 396 and name CB)	16.03	0.77	0.77
	assign (segid 3A4 and resid 224 and name N)	(segid 3A4 and resid 224 and name C)	2.45	0.03	0.02
60	assign (segid 3A4 and resid 224 and name N)	(segid 3A4 and resid 224 and name CB)	1.46	0.01	0.00
	assign (segid 3A4 and resid 224 and name N)	(segid 3A4 and resid 224 and name O)	2.46	0.03	0.02
	assign (segid 3A4 and resid 224 and name N)	(segid 3A4 and resid 224 and name O)	3.48	0.07	0.07
	assign (segid 3A4 and resid 224 and name N)	(segid 3A4 and resid 225 and name C)	4.80	0.05	0.05
	assign (segid 3A4 and resid 224 and name N)	(segid 3A4 and resid 225 and name CA)	4.23	0.04	0.04
	assign (segid 3A4 and resid 224 and name N)	(segid 3A4 and resid 225 and name CB)	4.95	0.05	0.06
65	assign (segid 3A4 and resid 224 and name N)	(segid 3A4 and resid 225 and name N)	2.82	0.05	0.05
	assign (segid 3A4 and resid 224 and name N)	(segid 3A4 and resid 225 and name O)	5.89	0.10	0.11
	assign (segid 3A4 and resid 224 and name N)	(segid 3A4 and resid 226 and name C)	5.57	0.09	0.10
	assign (segid 3A4 and resid 224 and name N)	(segid 3A4 and resid 226 and name CA)	5.47	0.06	0.06
	assign (segid 3A4 and resid 224 and name N)	(segid 3A4 and resid 226 and name N)	4.43	0.05	0.04
70	assign (segid 3A4 and resid 224 and name N)	(segid 3A4 and resid 226 and name O)	6.53	0.32	0.33
	assign (segid 3A4 and resid 224 and name O)	(segid 3A4 and resid 224 and name CB)	3.25	0.13	0.13
	assign (segid 3A4 and resid 224 and name O)	(segid 3A4 and resid 225 and name C)	3.00	0.14	0.14
	assign (segid 3A4 and resid 224 and name O)	(segid 3A4 and resid 225 and name CA)	2.79	0.02	0.03
	assign (segid 3A4 and resid 224 and name O)	(segid 3A4 and resid 225 and name CB)	4.27	0.02	0.01
75	assign (segid 3A4 and resid 224 and name O)	(segid 3A4 and resid 225 and name N)	2.25	0.01	0.00
	assign (segid 3A4 and resid 224 and name O)	(segid 3A4 and resid 225 and name O)	3.52	0.23	0.24
	assign (segid 3A4 and resid 224 and name O)	(segid 3A4 and resid 226 and name C)	4.20	0.35	0.35
	assign (segid 3A4 and resid 224 and name O)	(segid 3A4 and resid 226 and name CA)	4.35	0.26	0.26
	assign (segid 3A4 and resid 224 and name O)	(segid 3A4 and resid 226 and name N)	3.39	0.22	0.21
80	assign (segid 3A4 and resid 224 and name O)	(segid 3A4 and resid 226 and name O)	5.23	0.44	0.45
	assign (segid 3A4 and resid 224 and name O)	(segid 3A4 and resid 240 and name N)	7.42	0.29	0.29
	assign (segid 3A4 and resid 224 and name O)	(segid 3A4 and resid 244 and name CB)	5.82	0.83	0.83
	assign (segid 3A4 and resid 225 and name C)	(segid 3A4 and resid 225 and name CB)	2.48	0.03	0.03

	assign (segid 3A4 and resid 225 and name C) (segid 3A4 and resid 225 and name O)	1.24	0.01	0.01
	assign (segid 3A4 and resid 225 and name C) (segid 3A4 and resid 226 and name C)	3.28	0.11	0.10
	assign (segid 3A4 and resid 225 and name C) (segid 3A4 and resid 226 and name CA)	2.42	0.02	0.02
	assign (segid 3A4 and resid 225 and name C) (segid 3A4 and resid 226 and name N)	1.32	0.01	0.01
	assign (segid 3A4 and resid 225 and name C) (segid 3A4 and resid 226 and name O)	4.36	0.17	0.16
5	assign (segid 3A4 and resid 225 and name CA) (segid 3A4 and resid 225 and name C)	1.52	0.01	0.01
	assign (segid 3A4 and resid 225 and name CA) (segid 3A4 and resid 225 and name CB)	1.53	0.01	0.01
	assign (segid 3A4 and resid 225 and name CA) (segid 3A4 and resid 225 and name O)	2.40	0.02	0.02
	assign (segid 3A4 and resid 225 and name CA) (segid 3A4 and resid 226 and name C)	4.59	0.09	0.08
	assign (segid 3A4 and resid 225 and name CA) (segid 3A4 and resid 226 and name CA)	3.78	0.02	0.03
10	assign (segid 3A4 and resid 225 and name CA) (segid 3A4 and resid 226 and name N)	2.41	0.02	0.02
	assign (segid 3A4 and resid 225 and name CA) (segid 3A4 and resid 226 and name O)	5.71	0.14	0.14
	assign (segid 3A4 and resid 225 and name CA) (segid 3A4 and resid 240 and name CA)	8.84	0.52	0.52
	assign (segid 3A4 and resid 225 and name CA) (segid 3A4 and resid 240 and name CB)	10.33	0.50	0.51
	assign (segid 3A4 and resid 225 and name CA) (segid 3A4 and resid 241 and name CA)	8.23	0.62	0.62
15	assign (segid 3A4 and resid 225 and name CA) (segid 3A4 and resid 241 and name CB)	8.92	0.61	0.60
	assign (segid 3A4 and resid 225 and name CA) (segid 3A4 and resid 242 and name CA)	11.18	0.67	0.67
	assign (segid 3A4 and resid 225 and name CA) (segid 3A4 and resid 242 and name CB)	12.48	0.67	0.67
	assign (segid 3A4 and resid 225 and name CA) (segid 3A4 and resid 243 and name CA)	10.31	0.74	0.75
	assign (segid 3A4 and resid 225 and name CA) (segid 3A4 and resid 243 and name CB)	10.19	0.71	0.72
20	assign (segid 3A4 and resid 225 and name CA) (segid 3A4 and resid 244 and name CA)	7.26	0.87	0.87
	assign (segid 3A4 and resid 225 and name CA) (segid 3A4 and resid 244 and name CB)	6.04	0.90	0.90
	assign (segid 3A4 and resid 225 and name CA) (segid 3A4 and resid 245 and name CA)	9.99	0.89	0.89
	assign (segid 3A4 and resid 225 and name CA) (segid 3A4 and resid 245 and name CB)	10.80	0.85	0.86
	assign (segid 3A4 and resid 225 and name CA) (segid 3A4 and resid 246 and name CA)	12.58	0.94	0.94
25	assign (segid 3A4 and resid 225 and name CA) (segid 3A4 and resid 246 and name CB)	13.19	0.86	0.85
	assign (segid 3A4 and resid 225 and name CA) (segid 3A4 and resid 247 and name CA)	11.21	0.96	0.96
	assign (segid 3A4 and resid 225 and name CA) (segid 3A4 and resid 247 and name CB)	10.11	0.88	0.88
	assign (segid 3A4 and resid 225 and name CA) (segid 3A4 and resid 248 and name CA)	10.85	1.09	1.10
	assign (segid 3A4 and resid 225 and name CA) (segid 3A4 and resid 248 and name CB)	10.10	1.13	1.12
30	assign (segid 3A4 and resid 225 and name CA) (segid 3A4 and resid 249 and name CA)	14.30	1.08	1.08
	assign (segid 3A4 and resid 225 and name CA) (segid 3A4 and resid 250 and name CA)	15.68	1.02	1.02
	assign (segid 3A4 and resid 225 and name CA) (segid 3A4 and resid 250 and name CB)	15.44	0.98	0.97
	assign (segid 3A4 and resid 225 and name CA) (segid 3A4 and resid 251 and name CA)	14.85	1.08	1.07
	assign (segid 3A4 and resid 225 and name CA) (segid 3A4 and resid 251 and name CB)	13.56	1.09	1.10
35	assign (segid 3A4 and resid 225 and name CA) (segid 3A4 and resid 252 and name CA)	16.54	1.18	1.17
	assign (segid 3A4 and resid 225 and name CA) (segid 3A4 and resid 252 and name CB)	16.19	1.22	1.21
	assign (segid 3A4 and resid 225 and name CA) (segid 3A4 and resid 392 and name CA)	18.92	0.57	0.58
	assign (segid 3A4 and resid 225 and name CA) (segid 3A4 and resid 392 and name CB)	17.56	0.61	0.60
	assign (segid 3A4 and resid 225 and name CB) (segid 3A4 and resid 226 and name C)	5.56	0.14	0.14
40	assign (segid 3A4 and resid 225 and name CB) (segid 3A4 and resid 226 and name CA)	4.43	0.11	0.11
	assign (segid 3A4 and resid 225 and name CB) (segid 3A4 and resid 226 and name N)	3.12	0.12	0.13
	assign (segid 3A4 and resid 225 and name CB) (segid 3A4 and resid 226 and name O)	6.63	0.19	0.18
	assign (segid 3A4 and resid 225 and name CB) (segid 3A4 and resid 240 and name CA)	9.72	0.59	0.60
	assign (segid 3A4 and resid 225 and name CB) (segid 3A4 and resid 240 and name CB)	11.20	0.59	0.59
45	assign (segid 3A4 and resid 225 and name CB) (segid 3A4 and resid 241 and name CA)	8.58	0.75	0.76
	assign (segid 3A4 and resid 225 and name CB) (segid 3A4 and resid 241 and name CB)	9.07	0.75	0.74
	assign (segid 3A4 and resid 225 and name CB) (segid 3A4 and resid 242 and name CA)	11.63	0.79	0.80
	assign (segid 3A4 and resid 225 and name CB) (segid 3A4 and resid 242 and name CB)	12.98	0.80	0.79
	assign (segid 3A4 and resid 225 and name CB) (segid 3A4 and resid 243 and name CA)	11.16	0.80	0.79
50	assign (segid 3A4 and resid 225 and name CB) (segid 3A4 and resid 243 and name CB)	11.20	0.76	0.75
	assign (segid 3A4 and resid 225 and name CB) (segid 3A4 and resid 244 and name CA)	7.91	0.88	0.89
	assign (segid 3A4 and resid 225 and name CB) (segid 3A4 and resid 244 and name CB)	6.60	0.91	0.92
	assign (segid 3A4 and resid 225 and name CB) (segid 3A4 and resid 245 and name CA)	10.15	0.95	0.96
	assign (segid 3A4 and resid 225 and name CB) (segid 3A4 and resid 245 and name CB)	10.88	0.93	0.94
55	assign (segid 3A4 and resid 225 and name CB) (segid 3A4 and resid 246 and name CA)	13.06	0.98	0.98
	assign (segid 3A4 and resid 225 and name CB) (segid 3A4 and resid 246 and name CB)	13.79	0.90	0.89
	assign (segid 3A4 and resid 225 and name CB) (segid 3A4 and resid 247 and name CA)	11.86	0.94	0.94
	assign (segid 3A4 and resid 225 and name CB) (segid 3A4 and resid 247 and name CB)	10.88	0.84	0.83
	assign (segid 3A4 and resid 225 and name CB) (segid 3A4 and resid 248 and name CA)	11.03	1.11	1.10
60	assign (segid 3A4 and resid 225 and name CB) (segid 3A4 and resid 248 and name CB)	10.11	1.17	1.16
	assign (segid 3A4 and resid 225 and name CB) (segid 3A4 and resid 249 and name CA)	14.42	1.13	1.14
	assign (segid 3A4 and resid 225 and name CB) (segid 3A4 and resid 250 and name CA)	16.10	1.04	1.05
	assign (segid 3A4 and resid 225 and name CB) (segid 3A4 and resid 250 and name CB)	15.98	0.98	0.99
	assign (segid 3A4 and resid 225 and name CB) (segid 3A4 and resid 251 and name CA)	15.16	1.08	1.09
65	assign (segid 3A4 and resid 225 and name CB) (segid 3A4 and resid 251 and name CB)	13.87	1.09	1.09
	assign (segid 3A4 and resid 225 and name CB) (segid 3A4 and resid 252 and name CA)	16.53	1.23	1.22
	assign (segid 3A4 and resid 225 and name CB) (segid 3A4 and resid 252 and name CB)	16.08	1.27	1.27
	assign (segid 3A4 and resid 225 and name CB) (segid 3A4 and resid 392 and name CB)	18.41	0.53	0.52
	assign (segid 3A4 and resid 225 and name C) (segid 3A4 and resid 225 and name C)	2.47	0.02	0.02
70	assign (segid 3A4 and resid 225 and name N) (segid 3A4 and resid 225 and name CA)	1.46	0.01	0.01
	assign (segid 3A4 and resid 225 and name N) (segid 3A4 and resid 225 and name CB)	2.46	0.02	0.02
	assign (segid 3A4 and resid 225 and name N) (segid 3A4 and resid 225 and name O)	3.51	0.07	0.08
	assign (segid 3A4 and resid 225 and name N) (segid 3A4 and resid 226 and name C)	4.74	0.08	0.09
	assign (segid 3A4 and resid 225 and name N) (segid 3A4 and resid 226 and name CA)	4.20	0.06	0.06
75	assign (segid 3A4 and resid 225 and name N) (segid 3A4 and resid 226 and name N)	2.80	0.06	0.06
	assign (segid 3A4 and resid 225 and name N) (segid 3A4 and resid 226 and name O)	5.88	0.14	0.15
	assign (segid 3A4 and resid 225 and name N) (segid 3A4 and resid 244 and name CA)	6.96	0.64	0.63
	assign (segid 3A4 and resid 225 and name N) (segid 3A4 and resid 244 and name CB)	5.94	0.65	0.65
	assign (segid 3A4 and resid 225 and name O) (segid 3A4 and resid 225 and name CB)	3.26	0.09	0.09
80	assign (segid 3A4 and resid 225 and name O) (segid 3A4 and resid 226 and name C)	3.44	0.19	0.20
	assign (segid 3A4 and resid 225 and name O) (segid 3A4 and resid 226 and name CA)	2.77	0.05	0.04
	assign (segid 3A4 and resid 225 and name O) (segid 3A4 and resid 226 and name N)	2.25	0.02	0.03

	assign (segid 3A4 and resid 225 and name O)	(segid 3A4 and resid 226 and name O)	4.36	0.29	0.28
	assign (segid 3A4 and resid 226 and name C)	(segid 3A4 and resid 226 and name O)	1.24	0.02	0.01
	assign (segid 3A4 and resid 226 and name CA)	(segid 3A4 and resid 226 and name C)	1.52	0.01	0.00
	assign (segid 3A4 and resid 226 and name CA)	(segid 3A4 and resid 226 and name O)	2.38	0.02	0.03
5	assign (segid 3A4 and resid 226 and name CA)	(segid 3A4 and resid 240 and name CA)	10.85	0.81	0.81
	assign (segid 3A4 and resid 226 and name CA)	(segid 3A4 and resid 240 and name CB)	12.34	0.79	0.78
	assign (segid 3A4 and resid 226 and name CA)	(segid 3A4 and resid 241 and name CA)	11.17	0.76	0.76
	assign (segid 3A4 and resid 226 and name CA)	(segid 3A4 and resid 241 and name CB)	11.81	0.69	0.69
	assign (segid 3A4 and resid 226 and name CA)	(segid 3A4 and resid 242 and name CA)	14.28	0.79	0.79
10	assign (segid 3A4 and resid 226 and name CA)	(segid 3A4 and resid 242 and name CB)	12.43	0.83	0.84
	assign (segid 3A4 and resid 226 and name CA)	(segid 3A4 and resid 243 and name CA)	13.10	0.90	0.90
	assign (segid 3A4 and resid 226 and name CA)	(segid 3A4 and resid 243 and name CB)	12.63	0.92	0.92
	assign (segid 3A4 and resid 226 and name CA)	(segid 3A4 and resid 244 and name CA)	10.50	0.90	0.90
	assign (segid 3A4 and resid 226 and name CA)	(segid 3A4 and resid 244 and name CB)	9.40	0.95	0.94
15	assign (segid 3A4 and resid 226 and name CA)	(segid 3A4 and resid 245 and name CA)	13.58	0.88	0.88
	assign (segid 3A4 and resid 226 and name CA)	(segid 3A4 and resid 245 and name CB)	14.41	0.89	0.89
	assign (segid 3A4 and resid 226 and name CA)	(segid 3A4 and resid 246 and name CA)	15.88	0.92	0.93
	assign (segid 3A4 and resid 226 and name CA)	(segid 3A4 and resid 246 and name CB)	16.35	0.87	0.87
	assign (segid 3A4 and resid 226 and name CA)	(segid 3A4 and resid 247 and name CA)	14.16	0.91	0.91
20	assign (segid 3A4 and resid 226 and name CA)	(segid 3A4 and resid 247 and name CB)	12.88	0.86	0.85
	assign (segid 3A4 and resid 226 and name CA)	(segid 3A4 and resid 248 and name CA)	14.12	0.95	0.95
	assign (segid 3A4 and resid 226 and name CA)	(segid 3A4 and resid 248 and name CB)	13.52	0.99	0.99
	assign (segid 3A4 and resid 226 and name CA)	(segid 3A4 and resid 249 and name CA)	17.70	0.95	0.96
	assign (segid 3A4 and resid 226 and name CA)	(segid 3A4 and resid 251 and name CA)	17.56	0.90	0.90
25	assign (segid 3A4 and resid 226 and name CA)	(segid 3A4 and resid 251 and name CB)	16.20	0.92	0.91
	assign (segid 3A4 and resid 226 and name CA)	(segid 3A4 and resid 392 and name CB)	18.86	0.62	0.62
	assign (segid 3A4 and resid 226 and name N)	(segid 3A4 and resid 226 and name C)	2.48	0.02	0.02
	assign (segid 3A4 and resid 226 and name N)	(segid 3A4 and resid 226 and name CA)	1.46	0.02	0.01
	assign (segid 3A4 and resid 226 and name N)	(segid 3A4 and resid 226 and name O)	3.57	0.06	0.06
30	assign (segid 3A4 and resid 22 and name C)	(segid 3A4 and resid 22 and name O)	1.23	0.00	0.01
	assign (segid 3A4 and resid 22 and name C)	(segid 3A4 and resid 23 and name C)	3.47	0.06	0.07
	assign (segid 3A4 and resid 22 and name C)	(segid 3A4 and resid 23 and name CA)	2.44	0.02	0.02
	assign (segid 3A4 and resid 22 and name C)	(segid 3A4 and resid 23 and name CB)	3.49	0.08	0.08
	assign (segid 3A4 and resid 22 and name C)	(segid 3A4 and resid 23 and name N)	1.33	0.01	0.00
35	assign (segid 3A4 and resid 22 and name C)	(segid 3A4 and resid 23 and name O)	3.79	0.10	0.10
	assign (segid 3A4 and resid 22 and name C)	(segid 3A4 and resid 24 and name C)	6.80	0.12	0.12
	assign (segid 3A4 and resid 22 and name C)	(segid 3A4 and resid 24 and name CA)	5.70	0.17	0.16
	assign (segid 3A4 and resid 22 and name C)	(segid 3A4 and resid 24 and name CB)	6.25	0.34	0.33
	assign (segid 3A4 and resid 22 and name C)	(segid 3A4 and resid 24 and name N)	4.49	0.14	0.14
40	assign (segid 3A4 and resid 22 and name C)	(segid 3A4 and resid 24 and name O)	7.29	0.27	0.28
	assign (segid 3A4 and resid 22 and name C)	(segid 3A4 and resid 25 and name N)	7.43	0.36	0.36
	assign (segid 3A4 and resid 22 and name C)	(segid 3A4 and resid 29 and name C)	6.37	0.11	0.10
	assign (segid 3A4 and resid 22 and name C)	(segid 3A4 and resid 29 and name CA)	6.43	0.17	0.17
	assign (segid 3A4 and resid 22 and name C)	(segid 3A4 and resid 29 and name O)	7.44	0.12	0.12
45	assign (segid 3A4 and resid 22 and name C)	(segid 3A4 and resid 30 and name C)	4.71	0.08	0.08
	assign (segid 3A4 and resid 22 and name C)	(segid 3A4 and resid 30 and name CA)	5.74	0.07	0.07
	assign (segid 3A4 and resid 22 and name C)	(segid 3A4 and resid 30 and name N)	5.37	0.08	0.07
	assign (segid 3A4 and resid 22 and name C)	(segid 3A4 and resid 30 and name O)	3.58	0.08	0.08
	assign (segid 3A4 and resid 22 and name C)	(segid 3A4 and resid 31 and name C)	5.74	0.13	0.13
50	assign (segid 3A4 and resid 22 and name C)	(segid 3A4 and resid 31 and name CA)	5.11	0.18	0.18
	assign (segid 3A4 and resid 22 and name C)	(segid 3A4 and resid 31 and name CB)	6.15	0.29	0.28
	assign (segid 3A4 and resid 22 and name C)	(segid 3A4 and resid 31 and name N)	5.37	0.13	0.14
	assign (segid 3A4 and resid 22 and name C)	(segid 3A4 and resid 31 and name O)	6.75	0.14	0.15
	assign (segid 3A4 and resid 22 and name C)	(segid 3A4 and resid 32 and name C)	7.36	0.28	0.29
55	assign (segid 3A4 and resid 22 and name C)	(segid 3A4 and resid 32 and name CA)	6.51	0.28	0.29
	assign (segid 3A4 and resid 22 and name C)	(segid 3A4 and resid 32 and name CB)	6.15	0.36	0.37
	assign (segid 3A4 and resid 22 and name C)	(segid 3A4 and resid 32 and name N)	5.50	0.25	0.24
	assign (segid 3A4 and resid 22 and name C)	(segid 3A4 and resid 32 and name O)	7.04	0.33	0.33
	assign (segid 3A4 and resid 22 and name CA)	(segid 3A4 and resid 22 and name C)	1.52	0.01	0.01
60	assign (segid 3A4 and resid 22 and name CA)	(segid 3A4 and resid 22 and name O)	2.40	0.02	0.01
	assign (segid 3A4 and resid 22 and name CA)	(segid 3A4 and resid 23 and name C)	4.62	0.08	0.08
	assign (segid 3A4 and resid 22 and name CA)	(segid 3A4 and resid 23 and name CA)	3.80	0.02	0.03
	assign (segid 3A4 and resid 22 and name CA)	(segid 3A4 and resid 23 and name CB)	4.73	0.07	0.07
	assign (segid 3A4 and resid 22 and name CA)	(segid 3A4 and resid 23 and name N)	2.42	0.03	0.02
65	assign (segid 3A4 and resid 22 and name CA)	(segid 3A4 and resid 23 and name O)	4.60	0.12	0.12
	assign (segid 3A4 and resid 22 and name CA)	(segid 3A4 and resid 24 and name CA)	6.80	0.20	0.19
	assign (segid 3A4 and resid 22 and name CA)	(segid 3A4 and resid 24 and name CB)	7.32	0.44	0.44
	assign (segid 3A4 and resid 22 and name CA)	(segid 3A4 and resid 24 and name N)	5.73	0.15	0.16
	assign (segid 3A4 and resid 22 and name CA)	(segid 3A4 and resid 25 and name CA)	9.76	0.32	0.31
70	assign (segid 3A4 and resid 22 and name CA)	(segid 3A4 and resid 26 and name CA)	12.80	0.77	0.77
	assign (segid 3A4 and resid 22 and name CA)	(segid 3A4 and resid 29 and name C)	6.37	0.19	0.19
	assign (segid 3A4 and resid 22 and name CA)	(segid 3A4 and resid 29 and name CA)	6.63	0.22	0.22
	assign (segid 3A4 and resid 22 and name CA)	(segid 3A4 and resid 29 and name O)	7.29	0.20	0.21
	assign (segid 3A4 and resid 22 and name CA)	(segid 3A4 and resid 30 and name C)	4.34	0.13	0.14
75	assign (segid 3A4 and resid 22 and name CA)	(segid 3A4 and resid 30 and name CA)	5.54	0.13	0.14
	assign (segid 3A4 and resid 22 and name CA)	(segid 3A4 and resid 30 and name N)	5.38	0.16	0.17
	assign (segid 3A4 and resid 22 and name CA)	(segid 3A4 and resid 30 and name O)	3.38	0.12	0.12
	assign (segid 3A4 and resid 22 and name CA)	(segid 3A4 and resid 31 and name C)	5.09	0.23	0.24
	assign (segid 3A4 and resid 22 and name CA)	(segid 3A4 and resid 31 and name CA)	4.24	0.24	0.24
80	assign (segid 3A4 and resid 22 and name CA)	(segid 3A4 and resid 31 and name CB)	5.01	0.31	0.31
	assign (segid 3A4 and resid 22 and name CA)	(segid 3A4 and resid 31 and name N)	4.71	0.20	0.21
	assign (segid 3A4 and resid 22 and name CA)	(segid 3A4 and resid 31 and name O)	6.20	0.25	0.24
	assign (segid 3A4 and resid 22 and name CA)	(segid 3A4 and resid 322 and name CA)	13.72	0.13	0.13

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	assign	(segid 3A4 and resid 22 and name N)	(segid 3A4 and resid 30 and name N)	6.72	0.14	0.14
	assign	(segid 3A4 and resid 22 and name N)	(segid 3A4 and resid 30 and name O)	4.49	0.12	0.13
	assign	(segid 3A4 and resid 22 and name N)	(segid 3A4 and resid 31 and name C)	5.35	0.12	0.12
	assign	(segid 3A4 and resid 22 and name N)	(segid 3A4 and resid 31 and name CA)	4.69	0.13	0.12
5	assign	(segid 3A4 and resid 22 and name N)	(segid 3A4 and resid 31 and name CB)	5.25	0.23	0.24
	assign	(segid 3A4 and resid 22 and name N)	(segid 3A4 and resid 31 and name N)	5.50	0.10	0.11
	assign	(segid 3A4 and resid 22 and name N)	(segid 3A4 and resid 31 and name O)	6.53	0.11	0.12
	assign	(segid 3A4 and resid 22 and name N)	(segid 3A4 and resid 32 and name C)	6.40	0.26	0.25
	assign	(segid 3A4 and resid 22 and name N)	(segid 3A4 and resid 32 and name CA)	6.00	0.24	0.25
	assign	(segid 3A4 and resid 22 and name N)	(segid 3A4 and resid 32 and name CB)	5.97	0.31	0.31
10	assign	(segid 3A4 and resid 22 and name N)	(segid 3A4 and resid 32 and name N)	4.92	0.19	0.19
	assign	(segid 3A4 and resid 22 and name N)	(segid 3A4 and resid 32 and name O)	5.77	0.34	0.35
	assign	(segid 3A4 and resid 22 and name N)	(segid 3A4 and resid 23 and name C)	3.94	0.11	0.11
	assign	(segid 3A4 and resid 22 and name O)	(segid 3A4 and resid 23 and name CA)	2.79	0.03	0.03
15	assign	(segid 3A4 and resid 22 and name O)	(segid 3A4 and resid 23 and name CB)	3.81	0.14	0.14
	assign	(segid 3A4 and resid 22 and name O)	(segid 3A4 and resid 23 and name N)	2.25	0.01	0.01
	assign	(segid 3A4 and resid 22 and name O)	(segid 3A4 and resid 23 and name O)	4.54	0.13	0.12
	assign	(segid 3A4 and resid 22 and name O)	(segid 3A4 and resid 24 and name C)	7.05	0.20	0.20
	assign	(segid 3A4 and resid 22 and name O)	(segid 3A4 and resid 24 and name CA)	5.98	0.24	0.23
20	assign	(segid 3A4 and resid 22 and name O)	(segid 3A4 and resid 24 and name CB)	6.35	0.36	0.35
	assign	(segid 3A4 and resid 22 and name O)	(segid 3A4 and resid 24 and name N)	4.69	0.21	0.20
	assign	(segid 3A4 and resid 22 and name O)	(segid 3A4 and resid 29 and name C)	7.41	0.11	0.11
	assign	(segid 3A4 and resid 22 and name O)	(segid 3A4 and resid 29 and name CA)	7.32	0.20	0.21
	assign	(segid 3A4 and resid 22 and name O)	(segid 3A4 and resid 30 and name C)	5.92	0.08	0.09
25	assign	(segid 3A4 and resid 22 and name O)	(segid 3A4 and resid 30 and name N)	6.92	0.06	0.06
	assign	(segid 3A4 and resid 22 and name O)	(segid 3A4 and resid 30 and name O)	6.47	0.07	0.07
	assign	(segid 3A4 and resid 22 and name O)	(segid 3A4 and resid 31 and name C)	4.78	0.08	0.08
	assign	(segid 3A4 and resid 22 and name O)	(segid 3A4 and resid 31 and name CA)	6.75	0.16	0.17
	assign	(segid 3A4 and resid 22 and name O)	(segid 3A4 and resid 31 and name CB)	6.22	0.20	0.20
30	assign	(segid 3A4 and resid 22 and name O)	(segid 3A4 and resid 31 and name N)	7.20	0.30	0.31
	assign	(segid 3A4 and resid 22 and name O)	(segid 3A4 and resid 32 and name CA)	6.56	0.14	0.15
	assign	(segid 3A4 and resid 22 and name O)	(segid 3A4 and resid 32 and name CB)	7.25	0.38	0.38
	assign	(segid 3A4 and resid 22 and name O)	(segid 3A4 and resid 32 and name N)	6.72	0.46	0.45
	assign	(segid 3A4 and resid 22 and name O)	(segid 3A4 and resid 32 and name O)	6.35	0.31	0.31
35	assign	(segid 3A4 and resid 23 and name C)	(segid 3A4 and resid 23 and name CB)	2.50	0.03	0.02
	assign	(segid 3A4 and resid 23 and name C)	(segid 3A4 and resid 23 and name O)	1.24	0.01	0.01
	assign	(segid 3A4 and resid 23 and name C)	(segid 3A4 and resid 24 and name C)	3.42	0.07	0.07
	assign	(segid 3A4 and resid 23 and name C)	(segid 3A4 and resid 24 and name CA)	2.42	0.02	0.01
	assign	(segid 3A4 and resid 23 and name C)	(segid 3A4 and resid 24 and name CB)	3.45	0.10	0.09
40	assign	(segid 3A4 and resid 23 and name C)	(segid 3A4 and resid 24 and name N)	1.32	0.01	0.01
	assign	(segid 3A4 and resid 23 and name C)	(segid 3A4 and resid 24 and name O)	4.09	0.19	0.20
	assign	(segid 3A4 and resid 23 and name C)	(segid 3A4 and resid 25 and name C)	6.29	0.51	0.52
	assign	(segid 3A4 and resid 23 and name C)	(segid 3A4 and resid 25 and name CA)	5.32	0.28	0.29
	assign	(segid 3A4 and resid 23 and name C)	(segid 3A4 and resid 25 and name N)	4.03	0.31	0.32
45	assign	(segid 3A4 and resid 23 and name C)	(segid 3A4 and resid 25 and name O)	6.36	0.76	0.77
	assign	(segid 3A4 and resid 23 and name C)	(segid 3A4 and resid 29 and name C)	4.85	0.09	0.09
	assign	(segid 3A4 and resid 23 and name C)	(segid 3A4 and resid 29 and name CA)	4.50	0.18	0.18
	assign	(segid 3A4 and resid 23 and name C)	(segid 3A4 and resid 29 and name N)	5.44	0.24	0.23
50	assign	(segid 3A4 and resid 23 and name C)	(segid 3A4 and resid 29 and name O)	6.06	0.08	0.08
	assign	(segid 3A4 and resid 23 and name C)	(segid 3A4 and resid 30 and name C)	4.91	0.16	0.15
	assign	(segid 3A4 and resid 23 and name C)	(segid 3A4 and resid 30 and name CA)	5.04	0.17	0.18
	assign	(segid 3A4 and resid 23 and name C)	(segid 3A4 and resid 30 and name N)	4.13	0.11	0.12
	assign	(segid 3A4 and resid 23 and name C)	(segid 3A4 and resid 30 and name O)	4.01	0.08	0.08
55	assign	(segid 3A4 and resid 23 and name C)	(segid 3A4 and resid 31 and name C)	7.11	0.15	0.15
	assign	(segid 3A4 and resid 23 and name C)	(segid 3A4 and resid 31 and name CA)	6.60	0.19	0.18
	assign	(segid 3A4 and resid 23 and name C)	(segid 3A4 and resid 31 and name N)	6.09	0.18	0.19
	assign	(segid 3A4 and resid 23 and name C)	(segid 3A4 and resid 32 and name N)	7.22	0.29	0.29
	assign	(segid 3A4 and resid 23 and name CA)	(segid 3A4 and resid 23 and name C)	1.52	0.00	0.01
	assign	(segid 3A4 and resid 23 and name CA)	(segid 3A4 and resid 23 and name CB)	1.55	0.02	0.01
60	assign	(segid 3A4 and resid 23 and name CA)	(segid 3A4 and resid 23 and name O)	2.40	0.02	0.02
	assign	(segid 3A4 and resid 23 and name CA)	(segid 3A4 and resid 24 and name C)	4.65	0.07	0.07
	assign	(segid 3A4 and resid 23 and name CA)	(segid 3A4 and resid 24 and name CA)	3.79	0.01	0.02
	assign	(segid 3A4 and resid 23 and name CA)	(segid 3A4 and resid 24 and name CB)	4.67	0.08	0.08
	assign	(segid 3A4 and resid 23 and name CA)	(segid 3A4 and resid 24 and name N)	2.43	0.02	0.02
65	assign	(segid 3A4 and resid 23 and name CA)	(segid 3A4 and resid 24 and name O)	5.12	0.31	0.32
	assign	(segid 3A4 and resid 23 and name CA)	(segid 3A4 and resid 25 and name CA)	6.41	0.37	0.38
	assign	(segid 3A4 and resid 23 and name CA)	(segid 3A4 and resid 25 and name N)	5.25	0.40	0.41
	assign	(segid 3A4 and resid 23 and name CA)	(segid 3A4 and resid 26 and name CA)	9.65	0.73	0.73
	assign	(segid 3A4 and resid 23 and name CA)	(segid 3A4 and resid 29 and name C)	5.83	0.10	0.09
70	assign	(segid 3A4 and resid 23 and name CA)	(segid 3A4 and resid 29 and name CA)	5.71	0.16	0.16
	assign	(segid 3A4 and resid 23 and name CA)	(segid 3A4 and resid 29 and name N)	6.77	0.25	0.24
	assign	(segid 3A4 and resid 23 and name CA)	(segid 3A4 and resid 29 and name O)	7.00	0.09	0.09
	assign	(segid 3A4 and resid 23 and name CA)	(segid 3A4 and resid 30 and name C)	4.93	0.14	0.14
	assign	(segid 3A4 and resid 23 and name CA)	(segid 3A4 and resid 30 and name CA)	5.48	0.15	0.16
75	assign	(segid 3A4 and resid 23 and name CA)	(segid 3A4 and resid 30 and name N)	4.88	0.10	0.11
	assign	(segid 3A4 and resid 23 and name CA)	(segid 3A4 and resid 30 and name O)	3.84	0.09	0.10
	assign	(segid 3A4 and resid 23 and name CA)	(segid 3A4 and resid 31 and name C)	6.49	0.16	0.17
	assign	(segid 3A4 and resid 23 and name CA)	(segid 3A4 and resid 31 and name CA)	6.13	0.19	0.20
	assign	(segid 3A4 and resid 23 and name CA)	(segid 3A4 and resid 31 and name CB)	7.45	0.25	0.26
80	assign	(segid 3A4 and resid 23 and name CA)	(segid 3A4 and resid 31 and name N)	5.95	0.18	0.19
	assign	(segid 3A4 and resid 23 and name CA)	(segid 3A4 and resid 31 and name O)	7.22	0.20	0.21
	assign	(segid 3A4 and resid 23 and name CA)	(segid 3A4 and resid 32 and name CA)	13.57	0.17	0.17
	assign	(segid 3A4 and resid 23 and name CA)	(segid 3A4 and resid 323 and name CA)	14.64	0.23	0.22

	assign (segid 3A4 and resid 23 and name CA) (segid 3A4 and resid 323 and name CB)	14.98	0.36	0.35
	assign (segid 3A4 and resid 23 and name CA) (segid 3A4 and resid 324 and name CA)	14.70	0.26	0.27
	assign (segid 3A4 and resid 23 and name CA) (segid 3A4 and resid 324 and name CB)	15.35	0.37	0.37
	assign (segid 3A4 and resid 23 and name CA) (segid 3A4 and resid 325 and name CA)	15.87	0.32	0.33
5	assign (segid 3A4 and resid 23 and name CA) (segid 3A4 and resid 325 and name CB)	15.18	0.41	0.42
	assign (segid 3A4 and resid 23 and name CA) (segid 3A4 and resid 328 and name CA)	18.43	0.56	0.55
	assign (segid 3A4 and resid 23 and name CA) (segid 3A4 and resid 329 and name CA)	18.03	0.63	0.62
	assign (segid 3A4 and resid 23 and name CA) (segid 3A4 and resid 329 and name CB)	17.79	0.76	0.76
	assign (segid 3A4 and resid 23 and name CA) (segid 3A4 and resid 32 and name CA)	7.12	0.34	0.35
10	assign (segid 3A4 and resid 23 and name CA) (segid 3A4 and resid 32 and name CB)	6.46	0.41	0.42
	assign (segid 3A4 and resid 23 and name CA) (segid 3A4 and resid 32 and name N)	6.35	0.29	0.30
	assign (segid 3A4 and resid 23 and name CA) (segid 3A4 and resid 330 and name CA)	17.59	0.45	0.45
	assign (segid 3A4 and resid 23 and name CA) (segid 3A4 and resid 330 and name CB)	18.71	0.44	0.43
	assign (segid 3A4 and resid 23 and name CA) (segid 3A4 and resid 331 and name CA)	16.20	0.48	0.47
	assign (segid 3A4 and resid 23 and name CA) (segid 3A4 and resid 331 and name CB)	15.07	0.48	0.48
15	assign (segid 3A4 and resid 23 and name CA) (segid 3A4 and resid 332 and name CA)	17.18	0.76	0.75
	assign (segid 3A4 and resid 23 and name CA) (segid 3A4 and resid 335 and name CA)	14.10	0.38	0.39
	assign (segid 3A4 and resid 23 and name CA) (segid 3A4 and resid 336 and name CA)	14.92	0.31	0.31
	assign (segid 3A4 and resid 23 and name CA) (segid 3A4 and resid 336 and name CB)	15.75	0.26	0.25
20	assign (segid 3A4 and resid 23 and name CA) (segid 3A4 and resid 337 and name CA)	13.24	0.56	0.55
	assign (segid 3A4 and resid 23 and name CA) (segid 3A4 and resid 337 and name CB)	13.09	0.63	0.63
	assign (segid 3A4 and resid 23 and name CA) (segid 3A4 and resid 338 and name CA)	14.73	0.60	0.60
	assign (segid 3A4 and resid 23 and name CA) (segid 3A4 and resid 338 and name CB)	14.44	0.77	0.77
	assign (segid 3A4 and resid 23 and name CA) (segid 3A4 and resid 339 and name CA)	16.76	0.49	0.48
25	assign (segid 3A4 and resid 23 and name CA) (segid 3A4 and resid 339 and name CB)	18.19	0.47	0.47
	assign (segid 3A4 and resid 23 and name CA) (segid 3A4 and resid 33 and name CA)	10.70	0.33	0.33
	assign (segid 3A4 and resid 23 and name CA) (segid 3A4 and resid 33 and name CB)	11.78	0.32	0.32
	assign (segid 3A4 and resid 23 and name CA) (segid 3A4 and resid 340 and name CA)	15.25	0.31	0.31
30	assign (segid 3A4 and resid 23 and name CA) (segid 3A4 and resid 341 and name CA)	11.62	0.32	0.32
	assign (segid 3A4 and resid 23 and name CA) (segid 3A4 and resid 341 and name CB)	11.17	0.39	0.39
	assign (segid 3A4 and resid 23 and name CA) (segid 3A4 and resid 342 and name CA)	10.35	0.23	0.24
	assign (segid 3A4 and resid 23 and name CA) (segid 3A4 and resid 343 and name CA)	9.92	0.14	0.14
	assign (segid 3A4 and resid 23 and name CA) (segid 3A4 and resid 343 and name CB)	11.01	0.20	0.21
	assign (segid 3A4 and resid 23 and name CA) (segid 3A4 and resid 344 and name CA)	9.90	0.25	0.25
35	assign (segid 3A4 and resid 23 and name CA) (segid 3A4 and resid 344 and name CB)	8.90	0.29	0.29
	assign (segid 3A4 and resid 23 and name CA) (segid 3A4 and resid 345 and name CA)	12.59	0.36	0.36
	assign (segid 3A4 and resid 23 and name CA) (segid 3A4 and resid 345 and name CB)	13.91	0.34	0.35
	assign (segid 3A4 and resid 23 and name CA) (segid 3A4 and resid 346 and name CA)	13.04	0.45	0.45
	assign (segid 3A4 and resid 23 and name CA) (segid 3A4 and resid 346 and name CB)	12.21	0.49	0.49
40	assign (segid 3A4 and resid 23 and name CA) (segid 3A4 and resid 347 and name CA)	16.83	0.44	0.45
	assign (segid 3A4 and resid 23 and name CA) (segid 3A4 and resid 347 and name CB)	17.74	0.45	0.45
	assign (segid 3A4 and resid 23 and name CA) (segid 3A4 and resid 348 and name CA)	17.28	0.48	0.48
	assign (segid 3A4 and resid 23 and name CA) (segid 3A4 and resid 349 and name CA)	15.80	0.62	0.62
	assign (segid 3A4 and resid 23 and name CA) (segid 3A4 and resid 349 and name CB)	14.41	0.64	0.65
45	assign (segid 3A4 and resid 23 and name CA) (segid 3A4 and resid 34 and name CA)	12.39	0.46	0.46
	assign (segid 3A4 and resid 23 and name CA) (segid 3A4 and resid 34 and name CB)	11.85	0.50	0.51
	assign (segid 3A4 and resid 23 and name CA) (segid 3A4 and resid 350 and name CA)	18.02	0.83	0.83
	assign (segid 3A4 and resid 23 and name CA) (segid 3A4 and resid 350 and name CB)	18.21	0.94	0.95
	assign (segid 3A4 and resid 23 and name CA) (segid 3A4 and resid 35 and name CA)	15.76	0.43	0.43
50	assign (segid 3A4 and resid 23 and name CA) (segid 3A4 and resid 36 and name CA)	18.73	0.38	0.38
	assign (segid 3A4 and resid 23 and name CA) (segid 3A4 and resid 37 and name CA)	19.65	0.15	0.15
	assign (segid 3A4 and resid 23 and name CA) (segid 3A4 and resid 38 and name CA)	16.50	0.22	0.22
	assign (segid 3A4 and resid 23 and name CA) (segid 3A4 and resid 38 and name CB)	15.20	0.20	0.21
	assign (segid 3A4 and resid 23 and name CA) (segid 3A4 and resid 39 and name CA)	16.49	0.37	0.36
55	assign (segid 3A4 and resid 23 and name CA) (segid 3A4 and resid 39 and name CB)	16.48	0.37	0.38
	assign (segid 3A4 and resid 23 and name CA) (segid 3A4 and resid 41 and name CB)	19.28	0.35	0.35
	assign (segid 3A4 and resid 23 and name CA) (segid 3A4 and resid 42 and name CA)	17.26	0.40	0.40
	assign (segid 3A4 and resid 23 and name CA) (segid 3A4 and resid 42 and name CB)	15.83	0.40	0.40
	assign (segid 3A4 and resid 23 and name CA) (segid 3A4 and resid 431 and name CA)	17.09	0.90	0.90
60	assign (segid 3A4 and resid 23 and name CB) (segid 3A4 and resid 24 and name C)	4.90	0.20	0.19
	assign (segid 3A4 and resid 23 and name CB) (segid 3A4 and resid 24 and name CA)	4.45	0.12	0.12
	assign (segid 3A4 and resid 23 and name CB) (segid 3A4 and resid 24 and name CB)	5.56	0.10	0.10
	assign (segid 3A4 and resid 23 and name CB) (segid 3A4 and resid 24 and name N)	3.16	0.13	0.13
	assign (segid 3A4 and resid 23 and name CB) (segid 3A4 and resid 24 and name O)	5.25	0.49	0.48
65	assign (segid 3A4 and resid 23 and name CB) (segid 3A4 and resid 25 and name CA)	6.22	0.51	0.51
	assign (segid 3A4 and resid 23 and name CB) (segid 3A4 and resid 25 and name N)	5.30	0.50	0.49
	assign (segid 3A4 and resid 23 and name CB) (segid 3A4 and resid 26 and name CA)	9.55	0.90	0.91
	assign (segid 3A4 and resid 23 and name CB) (segid 3A4 and resid 29 and name C)	6.41	0.25	0.25
	assign (segid 3A4 and resid 23 and name CB) (segid 3A4 and resid 29 and name CA)	6.50	0.31	0.31
70	assign (segid 3A4 and resid 23 and name CB) (segid 3A4 and resid 30 and name C)	5.16	0.21	0.20
	assign (segid 3A4 and resid 23 and name CB) (segid 3A4 and resid 30 and name CA)	5.70	0.25	0.25
	assign (segid 3A4 and resid 23 and name CB) (segid 3A4 and resid 30 and name N)	5.36	0.23	0.23
	assign (segid 3A4 and resid 23 and name CB) (segid 3A4 and resid 30 and name O)	4.17	0.14	0.14
	assign (segid 3A4 and resid 23 and name CB) (segid 3A4 and resid 319 and name CA)	17.82	0.61	0.61
75	assign (segid 3A4 and resid 23 and name CB) (segid 3A4 and resid 319 and name CB)	18.52	0.48	0.47
	assign (segid 3A4 and resid 23 and name CB) (segid 3A4 and resid 31 and name C)	6.25	0.29	0.30
	assign (segid 3A4 and resid 23 and name CB) (segid 3A4 and resid 31 and name CA)	6.25	0.29	0.29
	assign (segid 3A4 and resid 23 and name CB) (segid 3A4 and resid 31 and name CB)	7.69	0.31	0.31
	assign (segid 3A4 and resid 23 and name CB) (segid 3A4 and resid 31 and name N)	6.10	0.28	0.28
80	assign (segid 3A4 and resid 23 and name CB) (segid 3A4 and resid 31 and name O)	6.84	0.32	0.32
	assign (segid 3A4 and resid 23 and name CB) (segid 3A4 and resid 322 and name CA)	12.80	0.27	0.27
	assign (segid 3A4 and resid 23 and name CB) (segid 3A4 and resid 323 and name CA)	14.21	0.25	0.24
	assign (segid 3A4 and resid 23 and name CB) (segid 3A4 and resid 323 and name CB)	14.56	0.36	0.37

	assign (segid 3A4 and resid 23 and name CB) (segid 3A4 and resid 324 and name CA)	14.65	0.21	0.21
	assign (segid 3A4 and resid 23 and name CB) (segid 3A4 and resid 324 and name CB)	15.32	0.29	0.28
	assign (segid 3A4 and resid 23 and name CB) (segid 3A4 and resid 325 and name CA)	16.09	0.30	0.30
	assign (segid 3A4 and resid 23 and name CB) (segid 3A4 and resid 325 and name CB)	15.51	0.41	0.40
5	assign (segid 3A4 and resid 23 and name CB) (segid 3A4 and resid 329 and name CA)	18.56	0.69	0.70
	assign (segid 3A4 and resid 23 and name CB) (segid 3A4 and resid 329 and name CB)	18.21	0.82	0.81
	assign (segid 3A4 and resid 23 and name CB) (segid 3A4 and resid 32 and name CA)	6.49	0.47	0.48
	assign (segid 3A4 and resid 23 and name CB) (segid 3A4 and resid 32 and name CB)	5.63	0.53	0.52
	assign (segid 3A4 and resid 23 and name CB) (segid 3A4 and resid 32 and name N)	6.01	0.43	0.42
10	assign (segid 3A4 and resid 23 and name CB) (segid 3A4 and resid 330 and name CA)	18.15	0.60	0.59
	assign (segid 3A4 and resid 23 and name CB) (segid 3A4 and resid 331 and name CA)	16.50	0.66	0.65
	assign (segid 3A4 and resid 23 and name CB) (segid 3A4 and resid 331 and name CB)	15.30	0.66	0.66
	assign (segid 3A4 and resid 23 and name CB) (segid 3A4 and resid 332 and name CA)	17.45	0.87	0.88
	assign (segid 3A4 and resid 23 and name CB) (segid 3A4 and resid 335 and name CA)	14.83	0.49	0.48
15	assign (segid 3A4 and resid 23 and name CB) (segid 3A4 and resid 336 and name CA)	15.76	0.35	0.34
	assign (segid 3A4 and resid 23 and name CB) (segid 3A4 and resid 336 and name CB)	16.68	0.27	0.27
	assign (segid 3A4 and resid 23 and name CB) (segid 3A4 and resid 337 and name CA)	13.95	0.58	0.59
	assign (segid 3A4 and resid 23 and name CB) (segid 3A4 and resid 337 and name CB)	13.66	0.68	0.67
	assign (segid 3A4 and resid 23 and name CB) (segid 3A4 and resid 338 and name CA)	15.57	0.57	0.57
20	assign (segid 3A4 and resid 23 and name CB) (segid 3A4 and resid 338 and name CB)	15.38	0.73	0.73
	assign (segid 3A4 and resid 23 and name CB) (segid 3A4 and resid 339 and name CA)	17.40	0.42	0.42
	assign (segid 3A4 and resid 23 and name CB) (segid 3A4 and resid 339 and name CB)	18.86	0.40	0.39
	assign (segid 3A4 and resid 23 and name CB) (segid 3A4 and resid 33 and name CA)	10.14	0.47	0.48
	assign (segid 3A4 and resid 23 and name CB) (segid 3A4 and resid 33 and name CB)	11.26	0.46	0.46
25	assign (segid 3A4 and resid 23 and name CB) (segid 3A4 and resid 340 and name CA)	15.73	0.19	0.20
	assign (segid 3A4 and resid 23 and name CB) (segid 3A4 and resid 341 and name CA)	12.12	0.23	0.24
	assign (segid 3A4 and resid 23 and name CB) (segid 3A4 and resid 341 and name CB)	11.76	0.34	0.33
	assign (segid 3A4 and resid 23 and name CB) (segid 3A4 and resid 342 and name CA)	10.38	0.18	0.19
	assign (segid 3A4 and resid 23 and name CB) (segid 3A4 and resid 343 and name CA)	9.64	0.22	0.22
30	assign (segid 3A4 and resid 23 and name CB) (segid 3A4 and resid 343 and name CB)	10.79	0.27	0.28
	assign (segid 3A4 and resid 23 and name CB) (segid 3A4 and resid 344 and name CA)	9.07	0.36	0.35
	assign (segid 3A4 and resid 23 and name CB) (segid 3A4 and resid 344 and name CB)	7.93	0.39	0.40
	assign (segid 3A4 and resid 23 and name CB) (segid 3A4 and resid 345 and name CA)	11.67	0.44	0.45
	assign (segid 3A4 and resid 23 and name CB) (segid 3A4 and resid 345 and name CB)	13.05	0.42	0.42
35	assign (segid 3A4 and resid 23 and name CB) (segid 3A4 and resid 346 and name CA)	11.84	0.53	0.54
	assign (segid 3A4 and resid 23 and name CB) (segid 3A4 and resid 346 and name CB)	11.00	0.59	0.58
	assign (segid 3A4 and resid 23 and name CB) (segid 3A4 and resid 347 and name CB)	15.63	0.53	0.53
	assign (segid 3A4 and resid 23 and name CB) (segid 3A4 and resid 347 and name CB)	16.52	0.53	0.53
	assign (segid 3A4 and resid 23 and name CB) (segid 3A4 and resid 348 and name CA)	15.95	0.56	0.56
40	assign (segid 3A4 and resid 23 and name CB) (segid 3A4 and resid 349 and name CA)	14.64	0.72	0.71
	assign (segid 3A4 and resid 23 and name CB) (segid 3A4 and resid 349 and name CB)	13.29	0.75	0.75
	assign (segid 3A4 and resid 23 and name CB) (segid 3A4 and resid 34 and name CA)	11.60	0.55	0.55
	assign (segid 3A4 and resid 23 and name CB) (segid 3A4 and resid 34 and name CB)	11.08	0.58	0.58
45	assign (segid 3A4 and resid 23 and name CB) (segid 3A4 and resid 350 and name CA)	16.99	0.91	0.92
	assign (segid 3A4 and resid 23 and name CB) (segid 3A4 and resid 350 and name CB)	17.20	1.04	1.05
	assign (segid 3A4 and resid 23 and name CB) (segid 3A4 and resid 35 and name CA)	15.12	0.54	0.53
	assign (segid 3A4 and resid 23 and name CB) (segid 3A4 and resid 36 and name CA)	17.99	0.51	0.51
	assign (segid 3A4 and resid 23 and name CB) (segid 3A4 and resid 37 and name CA)	19.18	0.31	0.30
50	assign (segid 3A4 and resid 23 and name CB) (segid 3A4 and resid 38 and name CA)	16.13	0.32	0.33
	assign (segid 3A4 and resid 23 and name CB) (segid 3A4 and resid 38 and name CB)	14.87	0.30	0.31
	assign (segid 3A4 and resid 23 and name CB) (segid 3A4 and resid 39 and name CA)	15.85	0.51	0.52
	assign (segid 3A4 and resid 23 and name CB) (segid 3A4 and resid 39 and name CB)	15.72	0.52	0.53
	assign (segid 3A4 and resid 23 and name CB) (segid 3A4 and resid 41 and name CB)	19.03	0.48	0.48
	assign (segid 3A4 and resid 23 and name CB) (segid 3A4 and resid 429 and name CA)	16.70	1.45	1.44
55	assign (segid 3A4 and resid 23 and name CB) (segid 3A4 and resid 42 and name CA)	16.93	0.56	0.56
	assign (segid 3A4 and resid 23 and name CB) (segid 3A4 and resid 42 and name CB)	15.46	0.56	0.56
	assign (segid 3A4 and resid 23 and name CB) (segid 3A4 and resid 430 and name CA)	14.69	1.77	1.76
	assign (segid 3A4 and resid 23 and name CB) (segid 3A4 and resid 431 and name CA)	15.73	0.90	0.89
	assign (segid 3A4 and resid 23 and name N) (segid 3A4 and resid 23 and name C)	2.38	0.02	0.03
60	assign (segid 3A4 and resid 23 and name N) (segid 3A4 and resid 23 and name CA)	1.46	0.01	0.00
	assign (segid 3A4 and resid 23 and name N) (segid 3A4 and resid 23 and name CB)	2.49	0.01	0.02
	assign (segid 3A4 and resid 23 and name N) (segid 3A4 and resid 23 and name O)	2.65	0.06	0.06
	assign (segid 3A4 and resid 23 and name N) (segid 3A4 and resid 24 and name C)	5.76	0.05	0.05
	assign (segid 3A4 and resid 23 and name N) (segid 3A4 and resid 24 and name CA)	4.75	0.07	0.06
65	assign (segid 3A4 and resid 23 and name N) (segid 3A4 and resid 24 and name CB)	5.54	0.23	0.22
	assign (segid 3A4 and resid 23 and name N) (segid 3A4 and resid 24 and name N)	3.55	0.05	0.05
	assign (segid 3A4 and resid 23 and name N) (segid 3A4 and resid 24 and name O)	6.32	0.26	0.27
	assign (segid 3A4 and resid 23 and name N) (segid 3A4 and resid 25 and name N)	6.29	0.35	0.34
	assign (segid 3A4 and resid 23 and name N) (segid 3A4 and resid 29 and name C)	5.46	0.07	0.07
70	assign (segid 3A4 and resid 23 and name N) (segid 3A4 and resid 29 and name CA)	5.55	0.11	0.12
	assign (segid 3A4 and resid 23 and name N) (segid 3A4 and resid 29 and name N)	6.80	0.14	0.15
	assign (segid 3A4 and resid 23 and name N) (segid 3A4 and resid 29 and name O)	6.57	0.09	0.09
	assign (segid 3A4 and resid 23 and name N) (segid 3A4 and resid 30 and name C)	4.01	0.10	0.09
	assign (segid 3A4 and resid 23 and name N) (segid 3A4 and resid 30 and name CA)	4.84	0.09	0.09
75	assign (segid 3A4 and resid 23 and name N) (segid 3A4 and resid 30 and name N)	4.41	0.05	0.05
	assign (segid 3A4 and resid 23 and name N) (segid 3A4 and resid 30 and name O)	2.84	0.07	0.08
	assign (segid 3A4 and resid 23 and name N) (segid 3A4 and resid 31 and name C)	5.47	0.10	0.10
	assign (segid 3A4 and resid 23 and name N) (segid 3A4 and resid 31 and name CA)	4.93	0.15	0.16
	assign (segid 3A4 and resid 23 and name N) (segid 3A4 and resid 31 and name CB)	6.16	0.24	0.25
80	assign (segid 3A4 and resid 23 and name N) (segid 3A4 and resid 31 and name N)	4.90	0.14	0.13
	assign (segid 3A4 and resid 23 and name N) (segid 3A4 and resid 31 and name O)	6.33	0.18	0.17
	assign (segid 3A4 and resid 23 and name N) (segid 3A4 and resid 32 and name C)	7.42	0.23	0.23
	assign (segid 3A4 and resid 23 and name N) (segid 3A4 and resid 32 and name CA)	6.34	0.24	0.25

	assign (segid 3A4 and resid 23 and name N) (segid 3A4 and resid 32 and name CB)	5.93	0.32	0.33
	assign (segid 3A4 and resid 23 and name N) (segid 3A4 and resid 32 and name N)	5.38	0.20	0.19
	assign (segid 3A4 and resid 23 and name N) (segid 3A4 and resid 32 and name O)	7.30	0.26	0.27
	assign (segid 3A4 and resid 23 and name N) (segid 3A4 and resid 342 and name O)	7.62	0.18	0.19
5	assign (segid 3A4 and resid 23 and name O) (segid 3A4 and resid 23 and name CB)	3.25	0.12	0.12
	assign (segid 3A4 and resid 23 and name O) (segid 3A4 and resid 24 and name C)	3.79	0.14	0.14
	assign (segid 3A4 and resid 23 and name O) (segid 3A4 and resid 24 and name CA)	2.76	0.05	0.05
	assign (segid 3A4 and resid 23 and name O) (segid 3A4 and resid 24 and name CB)	3.82	0.20	0.19
	assign (segid 3A4 and resid 23 and name O) (segid 3A4 and resid 24 and name N)	2.25	0.02	0.01
10	assign (segid 3A4 and resid 23 and name O) (segid 3A4 and resid 24 and name O)	4.64	0.16	0.16
	assign (segid 3A4 and resid 23 and name O) (segid 3A4 and resid 25 and name C)	6.31	0.60	0.59
	assign (segid 3A4 and resid 23 and name O) (segid 3A4 and resid 25 and name CA)	5.49	0.32	0.33
	assign (segid 3A4 and resid 23 and name O) (segid 3A4 and resid 25 and name N)	4.18	0.28	0.28
	assign (segid 3A4 and resid 23 and name O) (segid 3A4 and resid 25 and name O)	6.21	0.86	0.86
15	assign (segid 3A4 and resid 23 and name O) (segid 3A4 and resid 29 and name C)	3.63	0.09	0.09
	assign (segid 3A4 and resid 23 and name O) (segid 3A4 and resid 29 and name CA)	3.37	0.18	0.19
	assign (segid 3A4 and resid 23 and name O) (segid 3A4 and resid 29 and name N)	4.40	0.21	0.22
	assign (segid 3A4 and resid 23 and name O) (segid 3A4 and resid 29 and name O)	4.84	0.08	0.07
	assign (segid 3A4 and resid 23 and name O) (segid 3A4 and resid 30 and name C)	4.06	0.11	0.10
20	assign (segid 3A4 and resid 23 and name O) (segid 3A4 and resid 30 and name CA)	3.99	0.13	0.13
	assign (segid 3A4 and resid 23 and name O) (segid 3A4 and resid 30 and name N)	2.95	0.09	0.09
	assign (segid 3A4 and resid 23 and name O) (segid 3A4 and resid 30 and name O)	3.34	0.06	0.05
	assign (segid 3A4 and resid 23 and name O) (segid 3A4 and resid 31 and name C)	6.66	0.07	0.06
	assign (segid 3A4 and resid 23 and name O) (segid 3A4 and resid 31 and name CA)	6.01	0.14	0.15
25	assign (segid 3A4 and resid 23 and name O) (segid 3A4 and resid 31 and name CB)	7.25	0.23	0.23
	assign (segid 3A4 and resid 23 and name O) (segid 3A4 and resid 31 and name N)	5.30	0.13	0.14
	assign (segid 3A4 and resid 23 and name O) (segid 3A4 and resid 31 and name O)	7.17	0.17	0.18
	assign (segid 3A4 and resid 23 and name O) (segid 3A4 and resid 32 and name CB)	7.62	0.28	0.28
	assign (segid 3A4 and resid 23 and name O) (segid 3A4 and resid 32 and name N)	6.98	0.19	0.18
30	assign (segid 3A4 and resid 23 and name O) (segid 3A4 and resid 342 and name O)	7.32	0.25	0.24
	assign (segid 3A4 and resid 240 and name C) (segid 3A4 and resid 240 and name CB)	2.52	0.02	0.02
	assign (segid 3A4 and resid 240 and name C) (segid 3A4 and resid 240 and name O)	1.23	0.00	0.01
	assign (segid 3A4 and resid 240 and name C) (segid 3A4 and resid 241 and name C)	3.02	0.03	0.04
	assign (segid 3A4 and resid 240 and name C) (segid 3A4 and resid 241 and name CA)	2.44	0.01	0.00
35	assign (segid 3A4 and resid 240 and name C) (segid 3A4 and resid 241 and name CB)	3.69	0.02	0.03
	assign (segid 3A4 and resid 240 and name C) (segid 3A4 and resid 241 and name N)	1.32	0.01	0.01
	assign (segid 3A4 and resid 240 and name C) (segid 3A4 and resid 241 and name O)	3.95	0.07	0.06
	assign (segid 3A4 and resid 240 and name C) (segid 3A4 and resid 242 and name C)	4.54	0.06	0.07
	assign (segid 3A4 and resid 240 and name C) (segid 3A4 and resid 242 and name CA)	4.38	0.08	0.09
40	assign (segid 3A4 and resid 240 and name C) (segid 3A4 and resid 242 and name CB)	5.09	0.07	0.07
	assign (segid 3A4 and resid 240 and name C) (segid 3A4 and resid 242 and name N)	3.18	0.10	0.10
	assign (segid 3A4 and resid 240 and name C) (segid 3A4 and resid 242 and name O)	5.63	0.07	0.06
	assign (segid 3A4 and resid 240 and name C) (segid 3A4 and resid 243 and name C)	4.96	0.08	0.07
	assign (segid 3A4 and resid 240 and name C) (segid 3A4 and resid 243 and name CA)	4.63	0.10	0.11
45	assign (segid 3A4 and resid 240 and name C) (segid 3A4 and resid 243 and name CB)	4.49	0.17	0.18
	assign (segid 3A4 and resid 240 and name C) (segid 3A4 and resid 243 and name N)	3.85	0.07	0.07
	assign (segid 3A4 and resid 240 and name C) (segid 3A4 and resid 243 and name O)	6.16	0.07	0.07
	assign (segid 3A4 and resid 240 and name C) (segid 3A4 and resid 244 and name C)	6.18	0.16	0.16
	assign (segid 3A4 and resid 240 and name C) (segid 3A4 and resid 244 and name CA)	5.09	0.16	0.16
50	assign (segid 3A4 and resid 240 and name C) (segid 3A4 and resid 244 and name CB)	4.68	0.21	0.21
	assign (segid 3A4 and resid 240 and name C) (segid 3A4 and resid 244 and name N)	4.21	0.12	0.11
	assign (segid 3A4 and resid 240 and name C) (segid 3A4 and resid 244 and name O)	7.34	0.17	0.16
	assign (segid 3A4 and resid 240 and name C) (segid 3A4 and resid 245 and name CA)	7.31	0.18	0.19
	assign (segid 3A4 and resid 240 and name C) (segid 3A4 and resid 245 and name CB)	7.33	0.20	0.21
55	assign (segid 3A4 and resid 240 and name C) (segid 3A4 and resid 245 and name N)	6.04	0.18	0.19
	assign (segid 3A4 and resid 240 and name CA) (segid 3A4 and resid 240 and name C)	1.52	0.01	0.01
	assign (segid 3A4 and resid 240 and name CA) (segid 3A4 and resid 240 and name CB)	1.54	0.01	0.01
	assign (segid 3A4 and resid 240 and name CA) (segid 3A4 and resid 240 and name O)	2.40	0.02	0.01
	assign (segid 3A4 and resid 240 and name CA) (segid 3A4 and resid 241 and name C)	4.44	0.05	0.04
60	assign (segid 3A4 and resid 240 and name CA) (segid 3A4 and resid 241 and name CA)	3.81	0.02	0.01
	assign (segid 3A4 and resid 240 and name CA) (segid 3A4 and resid 241 and name CB)	4.83	0.05	0.04
	assign (segid 3A4 and resid 240 and name CA) (segid 3A4 and resid 241 and name N)	2.42	0.02	0.02
	assign (segid 3A4 and resid 240 and name CA) (segid 3A4 and resid 241 and name O)	5.42	0.07	0.07
	assign (segid 3A4 and resid 240 and name CA) (segid 3A4 and resid 242 and name C)	5.55	0.11	0.11
65	assign (segid 3A4 and resid 240 and name CA) (segid 3A4 and resid 242 and name CA)	5.42	0.09	0.10
	assign (segid 3A4 and resid 240 and name CA) (segid 3A4 and resid 242 and name CB)	5.80	0.12	0.12
	assign (segid 3A4 and resid 240 and name CA) (segid 3A4 and resid 242 and name N)	4.32	0.09	0.09
	assign (segid 3A4 and resid 240 and name CA) (segid 3A4 and resid 242 and name O)	6.69	0.10	0.10
	assign (segid 3A4 and resid 240 and name CA) (segid 3A4 and resid 243 and name C)	5.86	0.14	0.15
70	assign (segid 3A4 and resid 240 and name CA) (segid 3A4 and resid 243 and name CA)	5.31	0.17	0.17
	assign (segid 3A4 and resid 240 and name CA) (segid 3A4 and resid 243 and name CB)	4.76	0.23	0.24
	assign (segid 3A4 and resid 240 and name CA) (segid 3A4 and resid 243 and name N)	4.67	0.12	0.13
	assign (segid 3A4 and resid 240 and name CA) (segid 3A4 and resid 243 and name O)	7.05	0.14	0.14
	assign (segid 3A4 and resid 240 and name CA) (segid 3A4 and resid 244 and name C)	7.46	0.20	0.20
75	assign (segid 3A4 and resid 240 and name CA) (segid 3A4 and resid 244 and name CA)	6.27	0.22	0.21
	assign (segid 3A4 and resid 240 and name CA) (segid 3A4 and resid 244 and name CB)	5.93	0.26	0.26
	assign (segid 3A4 and resid 240 and name CA) (segid 3A4 and resid 244 and name N)	5.29	0.18	0.19
	assign (segid 3A4 and resid 240 and name CA) (segid 3A4 and resid 245 and name CA)	8.71	0.18	0.19
	assign (segid 3A4 and resid 240 and name CA) (segid 3A4 and resid 245 and name CB)	8.75	0.20	0.20
80	assign (segid 3A4 and resid 240 and name CA) (segid 3A4 and resid 245 and name N)	7.42	0.19	0.19
	assign (segid 3A4 and resid 240 and name CA) (segid 3A4 and resid 246 and name CA)	10.02	0.14	0.14
	assign (segid 3A4 and resid 240 and name CA) (segid 3A4 and resid 246 and name CB)	9.62	0.15	0.15
	assign (segid 3A4 and resid 240 and name CA) (segid 3A4 and resid 247 and name CA)	10.76	0.16	0.16

	assign (segid 3A4 and resid 240 and name CA)	(segid 3A4 and resid 247 and name CB)	10.06	0.18	0.19
	assign (segid 3A4 and resid 240 and name CA)	(segid 3A4 and resid 248 and name CA)	12.47	0.27	0.27
	assign (segid 3A4 and resid 240 and name CA)	(segid 3A4 and resid 248 and name CB)	12.07	0.33	0.34
	assign (segid 3A4 and resid 240 and name CA)	(segid 3A4 and resid 249 and name CA)	14.36	0.20	0.20
	assign (segid 3A4 and resid 240 and name CA)	(segid 3A4 and resid 250 and name CA)	15.48	0.11	0.11
5	assign (segid 3A4 and resid 240 and name CA)	(segid 3A4 and resid 250 and name CB)	14.80	0.20	0.21
	assign (segid 3A4 and resid 240 and name CA)	(segid 3A4 and resid 251 and name CA)	16.69	0.29	0.29
	assign (segid 3A4 and resid 240 and name CA)	(segid 3A4 and resid 251 and name CB)	16.02	0.38	0.37
	assign (segid 3A4 and resid 240 and name CA)	(segid 3A4 and resid 252 and name CA)	18.63	0.32	0.33
	assign (segid 3A4 and resid 240 and name CA)	(segid 3A4 and resid 252 and name CB)	18.17	0.35	0.35
10	assign (segid 3A4 and resid 240 and name CA)	(segid 3A4 and resid 241 and name C)	4.79	0.05	0.06
	assign (segid 3A4 and resid 240 and name CB)	(segid 3A4 and resid 241 and name CA)	4.48	0.06	0.06
	assign (segid 3A4 and resid 240 and name CB)	(segid 3A4 and resid 241 and name CB)	5.34	0.14	0.13
	assign (segid 3A4 and resid 240 and name CB)	(segid 3A4 and resid 241 and name N)	3.15	0.10	0.11
	assign (segid 3A4 and resid 240 and name CB)	(segid 3A4 and resid 241 and name O)	5.87	0.08	0.09
15	assign (segid 3A4 and resid 240 and name CB)	(segid 3A4 and resid 242 and name C)	5.35	0.14	0.15
	assign (segid 3A4 and resid 240 and name CB)	(segid 3A4 and resid 242 and name CA)	5.12	0.13	0.12
	assign (segid 3A4 and resid 240 and name CB)	(segid 3A4 and resid 242 and name CB)	5.09	0.17	0.17
	assign (segid 3A4 and resid 240 and name CB)	(segid 3A4 and resid 242 and name N)	4.24	0.08	0.08
	assign (segid 3A4 and resid 240 and name CB)	(segid 3A4 and resid 242 and name O)	6.55	0.15	0.15
20	assign (segid 3A4 and resid 240 and name CB)	(segid 3A4 and resid 243 and name C)	6.18	0.19	0.20
	assign (segid 3A4 and resid 240 and name CB)	(segid 3A4 and resid 243 and name CA)	5.28	0.22	0.22
	assign (segid 3A4 and resid 240 and name CB)	(segid 3A4 and resid 243 and name CB)	4.73	0.25	0.25
	assign (segid 3A4 and resid 240 and name CB)	(segid 3A4 and resid 243 and name N)	4.52	0.19	0.19
	assign (segid 3A4 and resid 240 and name CB)	(segid 3A4 and resid 243 and name O)	7.36	0.19	0.19
25	assign (segid 3A4 and resid 240 and name CB)	(segid 3A4 and resid 244 and name CA)	7.08	0.23	0.22
	assign (segid 3A4 and resid 240 and name CB)	(segid 3A4 and resid 244 and name CB)	6.98	0.24	0.23
	assign (segid 3A4 and resid 240 and name CB)	(segid 3A4 and resid 244 and name N)	5.89	0.21	0.22
	assign (segid 3A4 and resid 240 and name CB)	(segid 3A4 and resid 245 and name CA)	9.14	0.18	0.18
	assign (segid 3A4 and resid 240 and name CB)	(segid 3A4 and resid 245 and name CB)	9.03	0.21	0.21
30	assign (segid 3A4 and resid 240 and name CB)	(segid 3A4 and resid 246 and name CA)	10.06	0.17	0.18
	assign (segid 3A4 and resid 240 and name CB)	(segid 3A4 and resid 246 and name CB)	9.46	0.20	0.21
	assign (segid 3A4 and resid 240 and name CB)	(segid 3A4 and resid 247 and name CA)	11.18	0.16	0.16
	assign (segid 3A4 and resid 240 and name CB)	(segid 3A4 and resid 247 and name CB)	10.62	0.20	0.20
	assign (segid 3A4 and resid 240 and name CB)	(segid 3A4 and resid 248 and name CA)	13.13	0.25	0.25
35	assign (segid 3A4 and resid 240 and name CB)	(segid 3A4 and resid 248 and name CB)	12.81	0.30	0.30
	assign (segid 3A4 and resid 240 and name CB)	(segid 3A4 and resid 249 and name CA)	14.68	0.21	0.20
	assign (segid 3A4 and resid 240 and name CB)	(segid 3A4 and resid 250 and name CA)	15.72	0.13	0.12
	assign (segid 3A4 and resid 240 and name CB)	(segid 3A4 and resid 250 and name CB)	15.00	0.21	0.21
	assign (segid 3A4 and resid 240 and name CB)	(segid 3A4 and resid 251 and name CA)	17.24	0.26	0.26
40	assign (segid 3A4 and resid 240 and name CB)	(segid 3A4 and resid 251 and name CB)	16.68	0.35	0.36
	assign (segid 3A4 and resid 240 and name CB)	(segid 3A4 and resid 252 and name CA)	19.16	0.30	0.31
	assign (segid 3A4 and resid 240 and name CB)	(segid 3A4 and resid 252 and name CB)	18.69	0.34	0.34
	assign (segid 3A4 and resid 240 and name N)	(segid 3A4 and resid 240 and name C)	2.40	0.04	0.04
	assign (segid 3A4 and resid 240 and name N)	(segid 3A4 and resid 240 and name CA)	1.45	0.00	0.01
45	assign (segid 3A4 and resid 240 and name N)	(segid 3A4 and resid 240 and name CB)	2.47	0.04	0.03
	assign (segid 3A4 and resid 240 and name N)	(segid 3A4 and resid 240 and name O)	2.66	0.05	0.05
	assign (segid 3A4 and resid 240 and name N)	(segid 3A4 and resid 241 and name C)	5.32	0.08	0.08
	assign (segid 3A4 and resid 240 and name N)	(segid 3A4 and resid 241 and name CA)	4.80	0.07	0.07
	assign (segid 3A4 and resid 240 and name N)	(segid 3A4 and resid 241 and name CB)	5.99	0.06	0.07
50	assign (segid 3A4 and resid 240 and name N)	(segid 3A4 and resid 241 and name N)	3.58	0.06	0.06
	assign (segid 3A4 and resid 240 and name N)	(segid 3A4 and resid 241 and name O)	6.12	0.12	0.12
	assign (segid 3A4 and resid 240 and name N)	(segid 3A4 and resid 242 and name C)	6.02	0.16	0.16
	assign (segid 3A4 and resid 240 and name N)	(segid 3A4 and resid 242 and name CA)	6.23	0.11	0.11
	assign (segid 3A4 and resid 240 and name N)	(segid 3A4 and resid 242 and name CB)	6.68	0.10	0.11
55	assign (segid 3A4 and resid 240 and name N)	(segid 3A4 and resid 242 and name N)	5.29	0.11	0.11
	assign (segid 3A4 and resid 240 and name N)	(segid 3A4 and resid 242 and name O)	7.06	0.18	0.18
	assign (segid 3A4 and resid 240 and name N)	(segid 3A4 and resid 243 and name C)	5.63	0.23	0.23
	assign (segid 3A4 and resid 240 and name N)	(segid 3A4 and resid 243 and name CA)	5.18	0.24	0.24
	assign (segid 3A4 and resid 240 and name N)	(segid 3A4 and resid 243 and name CB)	4.31	0.31	0.32
60	assign (segid 3A4 and resid 240 and name N)	(segid 3A4 and resid 243 and name N)	4.94	0.17	0.17
	assign (segid 3A4 and resid 240 and name N)	(segid 3A4 and resid 243 and name O)	6.71	0.22	0.22
	assign (segid 3A4 and resid 240 and name N)	(segid 3A4 and resid 244 and name C)	7.39	0.30	0.30
	assign (segid 3A4 and resid 240 and name N)	(segid 3A4 and resid 244 and name CA)	6.04	0.33	0.32
	assign (segid 3A4 and resid 240 and name N)	(segid 3A4 and resid 244 and name CB)	5.82	0.35	0.36
65	assign (segid 3A4 and resid 240 and name N)	(segid 3A4 and resid 244 and name N)	5.13	0.27	0.28
	assign (segid 3A4 and resid 240 and name N)	(segid 3A4 and resid 245 and name N)	7.59	0.26	0.26
	assign (segid 3A4 and resid 240 and name O)	(segid 3A4 and resid 240 and name CB)	3.31	0.10	0.11
	assign (segid 3A4 and resid 240 and name O)	(segid 3A4 and resid 241 and name C)	2.95	0.08	0.07
	assign (segid 3A4 and resid 240 and name O)	(segid 3A4 and resid 241 and name CA)	2.78	0.02	0.02
70	assign (segid 3A4 and resid 240 and name O)	(segid 3A4 and resid 241 and name CB)	4.25	0.02	0.02
	assign (segid 3A4 and resid 240 and name O)	(segid 3A4 and resid 241 and name N)	2.25	0.01	0.01
	assign (segid 3A4 and resid 240 and name O)	(segid 3A4 and resid 241 and name O)	3.55	0.09	0.09
	assign (segid 3A4 and resid 240 and name O)	(segid 3A4 and resid 242 and name C)	3.98	0.15	0.15
	assign (segid 3A4 and resid 240 and name O)	(segid 3A4 and resid 242 and name CA)	4.20	0.19	0.19
75	assign (segid 3A4 and resid 240 and name O)	(segid 3A4 and resid 242 and name CB)	5.12	0.14	0.14
	assign (segid 3A4 and resid 240 and name O)	(segid 3A4 and resid 242 and name N)	3.24	0.20	0.20
	assign (segid 3A4 and resid 240 and name O)	(segid 3A4 and resid 242 and name O)	4.93	0.14	0.15
	assign (segid 3A4 and resid 240 and name O)	(segid 3A4 and resid 243 and name C)	3.84	0.05	0.05
	assign (segid 3A4 and resid 240 and name O)	(segid 3A4 and resid 243 and name CA)	3.73	0.05	0.05
80	assign (segid 3A4 and resid 240 and name O)	(segid 3A4 and resid 243 and name CB)	3.66	0.14	0.14
	assign (segid 3A4 and resid 240 and name O)	(segid 3A4 and resid 243 and name N)	3.19	0.12	0.12
	assign (segid 3A4 and resid 240 and name O)	(segid 3A4 and resid 243 and name O)	5.02	0.05	0.05

	assign (segid 3A4 and resid 240 and name O) (segid 3A4 and resid 244 and name C)	5.09	0.19	0.19
	assign (segid 3A4 and resid 240 and name O) (segid 3A4 and resid 244 and name CA)	3.94	0.19	0.18
	assign (segid 3A4 and resid 240 and name O) (segid 3A4 and resid 244 and name CB)	3.69	0.24	0.24
	assign (segid 3A4 and resid 240 and name O) (segid 3A4 and resid 244 and name N)	3.03	0.12	0.13
	assign (segid 3A4 and resid 240 and name O) (segid 3A4 and resid 244 and name O)	6.22	0.20	0.19
5	assign (segid 3A4 and resid 240 and name O) (segid 3A4 and resid 245 and name C)	7.27	0.15	0.15
	assign (segid 3A4 and resid 240 and name O) (segid 3A4 and resid 245 and name CA)	6.45	0.20	0.19
	assign (segid 3A4 and resid 240 and name O) (segid 3A4 and resid 245 and name CB)	6.66	0.19	0.20
	assign (segid 3A4 and resid 240 and name O) (segid 3A4 and resid 245 and name N)	5.10	0.20	0.20
	assign (segid 3A4 and resid 240 and name O) (segid 3A4 and resid 246 and name CB)	7.81	0.06	0.05
10	assign (segid 3A4 and resid 240 and name O) (segid 3A4 and resid 246 and name N)	6.92	0.11	0.11
	assign (segid 3A4 and resid 241 and name C) (segid 3A4 and resid 241 and name CB)	2.47	0.03	0.03
	assign (segid 3A4 and resid 241 and name C) (segid 3A4 and resid 241 and name O)	1.23	0.00	0.01
	assign (segid 3A4 and resid 241 and name C) (segid 3A4 and resid 242 and name C)	3.08	0.08	0.09
	assign (segid 3A4 and resid 241 and name C) (segid 3A4 and resid 242 and name CA)	2.43	0.02	0.02
15	assign (segid 3A4 and resid 241 and name C) (segid 3A4 and resid 242 and name CB)	3.67	0.03	0.04
	assign (segid 3A4 and resid 241 and name C) (segid 3A4 and resid 242 and name O)	1.33	0.01	0.00
	assign (segid 3A4 and resid 241 and name C) (segid 3A4 and resid 242 and name N)	3.90	0.12	0.12
	assign (segid 3A4 and resid 241 and name C) (segid 3A4 and resid 243 and name C)	4.62	0.15	0.15
	assign (segid 3A4 and resid 241 and name C) (segid 3A4 and resid 243 and name CA)	4.57	0.16	0.15
20	assign (segid 3A4 and resid 241 and name C) (segid 3A4 and resid 243 and name CB)	5.35	0.16	0.17
	assign (segid 3A4 and resid 241 and name C) (segid 3A4 and resid 243 and name N)	3.38	0.14	0.14
	assign (segid 3A4 and resid 241 and name C) (segid 3A4 and resid 244 and name C)	4.93	0.15	0.15
	assign (segid 3A4 and resid 241 and name C) (segid 3A4 and resid 244 and name CA)	4.57	0.09	0.10
25	assign (segid 3A4 and resid 241 and name C) (segid 3A4 and resid 244 and name CB)	4.28	0.12	0.11
	assign (segid 3A4 and resid 241 and name C) (segid 3A4 and resid 244 and name N)	3.88	0.12	0.12
	assign (segid 3A4 and resid 241 and name C) (segid 3A4 and resid 244 and name O)	6.14	0.15	0.15
	assign (segid 3A4 and resid 241 and name C) (segid 3A4 and resid 245 and name C)	6.19	0.25	0.24
	assign (segid 3A4 and resid 241 and name C) (segid 3A4 and resid 245 and name CA)	5.11	0.23	0.22
30	assign (segid 3A4 and resid 241 and name C) (segid 3A4 and resid 245 and name CB)	4.71	0.25	0.25
	assign (segid 3A4 and resid 241 and name C) (segid 3A4 and resid 245 and name N)	4.20	0.19	0.20
	assign (segid 3A4 and resid 241 and name C) (segid 3A4 and resid 245 and name O)	7.35	0.24	0.25
	assign (segid 3A4 and resid 241 and name C) (segid 3A4 and resid 246 and name CA)	7.35	0.24	0.25
	assign (segid 3A4 and resid 241 and name C) (segid 3A4 and resid 246 and name CB)	7.38	0.24	0.24
35	assign (segid 3A4 and resid 241 and name C) (segid 3A4 and resid 246 and name N)	6.07	0.25	0.24
	assign (segid 3A4 and resid 241 and name CA) (segid 3A4 and resid 241 and name CB)	1.52	0.01	0.01
	assign (segid 3A4 and resid 241 and name CA) (segid 3A4 and resid 241 and name O)	1.51	0.01	0.02
	assign (segid 3A4 and resid 241 and name CA) (segid 3A4 and resid 241 and name N)	2.40	0.02	0.02
	assign (segid 3A4 and resid 241 and name CA) (segid 3A4 and resid 242 and name C)	4.46	0.08	0.07
40	assign (segid 3A4 and resid 241 and name CA) (segid 3A4 and resid 242 and name CA)	3.80	0.01	0.02
	assign (segid 3A4 and resid 241 and name CA) (segid 3A4 and resid 242 and name CB)	4.82	0.05	0.05
	assign (segid 3A4 and resid 241 and name CA) (segid 3A4 and resid 242 and name N)	2.43	0.03	0.03
	assign (segid 3A4 and resid 241 and name CA) (segid 3A4 and resid 242 and name O)	5.34	0.11	0.12
	assign (segid 3A4 and resid 241 and name CA) (segid 3A4 and resid 243 and name C)	5.54	0.14	0.14
45	assign (segid 3A4 and resid 241 and name CA) (segid 3A4 and resid 243 and name CA)	5.53	0.14	0.15
	assign (segid 3A4 and resid 241 and name CA) (segid 3A4 and resid 243 and name CB)	6.01	0.17	0.17
	assign (segid 3A4 and resid 241 and name CA) (segid 3A4 and resid 243 and name N)	4.46	0.13	0.12
	assign (segid 3A4 and resid 241 and name CA) (segid 3A4 and resid 243 and name O)	6.66	0.14	0.15
	assign (segid 3A4 and resid 241 and name CA) (segid 3A4 and resid 244 and name C)	5.75	0.17	0.17
50	assign (segid 3A4 and resid 241 and name CA) (segid 3A4 and resid 244 and name CA)	5.13	0.08	0.08
	assign (segid 3A4 and resid 241 and name CA) (segid 3A4 and resid 244 and name CB)	4.43	0.05	0.05
	assign (segid 3A4 and resid 241 and name CA) (segid 3A4 and resid 244 and name N)	4.59	0.11	0.12
	assign (segid 3A4 and resid 241 and name CA) (segid 3A4 and resid 244 and name O)	6.95	0.17	0.18
	assign (segid 3A4 and resid 241 and name CA) (segid 3A4 and resid 245 and name C)	7.44	0.26	0.25
55	assign (segid 3A4 and resid 241 and name CA) (segid 3A4 and resid 245 and name CA)	6.25	0.26	0.25
	assign (segid 3A4 and resid 241 and name CA) (segid 3A4 and resid 245 and name CB)	5.95	0.29	0.28
	assign (segid 3A4 and resid 241 and name CA) (segid 3A4 and resid 245 and name N)	5.23	0.21	0.22
	assign (segid 3A4 and resid 241 and name CA) (segid 3A4 and resid 246 and name CA)	8.71	0.23	0.23
	assign (segid 3A4 and resid 241 and name CA) (segid 3A4 and resid 246 and name CB)	8.76	0.22	0.22
60	assign (segid 3A4 and resid 241 and name CA) (segid 3A4 and resid 246 and name N)	7.40	0.24	0.25
	assign (segid 3A4 and resid 241 and name CA) (segid 3A4 and resid 247 and name CA)	10.02	0.20	0.20
	assign (segid 3A4 and resid 241 and name CA) (segid 3A4 and resid 247 and name CB)	9.64	0.20	0.21
	assign (segid 3A4 and resid 241 and name CA) (segid 3A4 and resid 248 and name CA)	10.68	0.17	0.17
	assign (segid 3A4 and resid 241 and name CA) (segid 3A4 and resid 248 and name CB)	9.93	0.19	0.18
65	assign (segid 3A4 and resid 241 and name CA) (segid 3A4 and resid 249 and name CA)	12.38	0.21	0.20
	assign (segid 3A4 and resid 241 and name CA) (segid 3A4 and resid 250 and name CA)	14.33	0.26	0.26
	assign (segid 3A4 and resid 241 and name CA) (segid 3A4 and resid 250 and name CB)	14.01	0.36	0.36
	assign (segid 3A4 and resid 241 and name CA) (segid 3A4 and resid 251 and name CA)	15.49	0.13	0.14
	assign (segid 3A4 and resid 241 and name CA) (segid 3A4 and resid 251 and name CB)	14.83	0.19	0.19
70	assign (segid 3A4 and resid 241 and name CA) (segid 3A4 and resid 252 and name CA)	16.75	0.23	0.23
	assign (segid 3A4 and resid 241 and name CA) (segid 3A4 and resid 252 and name CB)	16.04	0.30	0.29
	assign (segid 3A4 and resid 241 and name CA) (segid 3A4 and resid 253 and name CA)	18.51	0.14	0.15
	assign (segid 3A4 and resid 241 and name CB) (segid 3A4 and resid 242 and name C)	5.46	0.10	0.10
75	assign (segid 3A4 and resid 241 and name CB) (segid 3A4 and resid 242 and name CA)	4.47	0.06	0.06
	assign (segid 3A4 and resid 241 and name CB) (segid 3A4 and resid 242 and name CB)	5.29	0.11	0.10
	assign (segid 3A4 and resid 241 and name CB) (segid 3A4 and resid 242 and name N)	3.17	0.08	0.08
	assign (segid 3A4 and resid 241 and name CB) (segid 3A4 and resid 242 and name O)	6.30	0.15	0.15
	assign (segid 3A4 and resid 241 and name CB) (segid 3A4 and resid 243 and name C)	6.93	0.17	0.16
	assign (segid 3A4 and resid 241 and name CB) (segid 3A4 and resid 243 and name CA)	6.87	0.14	0.15
80	assign (segid 3A4 and resid 241 and name CB) (segid 3A4 and resid 243 and name CB)	7.41	0.16	0.16
	assign (segid 3A4 and resid 241 and name CB) (segid 3A4 and resid 243 and name N)	5.68	0.12	0.11
	assign (segid 3A4 and resid 241 and name CB) (segid 3A4 and resid 244 and name C)	6.89	0.23	0.24

	assign (segid 3A4 and resid 241 and name CB)	(segid 3A4 and resid 244 and name CA)	6.45	0.13	0.13
	assign (segid 3A4 and resid 241 and name CB)	(segid 3A4 and resid 244 and name CB)	5.65	0.12	0.12
	assign (segid 3A4 and resid 241 and name CB)	(segid 3A4 and resid 244 and name N)	6.00	0.15	0.15
	assign (segid 3A4 and resid 241 and name CB)	(segid 3A4 and resid 245 and name CA)	7.01	0.33	0.32
5	assign (segid 3A4 and resid 241 and name CB)	(segid 3A4 and resid 245 and name CB)	6.44	0.38	0.38
	assign (segid 3A4 and resid 241 and name CB)	(segid 3A4 and resid 245 and name N)	6.21	0.27	0.27
	assign (segid 3A4 and resid 241 and name CB)	(segid 3A4 and resid 246 and name CA)	9.70	0.32	0.31
	assign (segid 3A4 and resid 241 and name CB)	(segid 3A4 and resid 246 and name CB)	9.80	0.30	0.29
	assign (segid 3A4 and resid 241 and name CB)	(segid 3A4 and resid 247 and name CA)	11.26	0.26	0.26
10	assign (segid 3A4 and resid 241 and name CB)	(segid 3A4 and resid 247 and name CB)	10.97	0.27	0.27
	assign (segid 3A4 and resid 241 and name CB)	(segid 3A4 and resid 248 and name CA)	11.63	0.20	0.21
	assign (segid 3A4 and resid 241 and name CB)	(segid 3A4 and resid 248 and name CB)	10.75	0.17	0.17
	assign (segid 3A4 and resid 241 and name CB)	(segid 3A4 and resid 249 and name CA)	13.17	0.29	0.28
	assign (segid 3A4 and resid 241 and name CB)	(segid 3A4 and resid 250 and name CA)	15.38	0.34	0.35
15	assign (segid 3A4 and resid 241 and name CB)	(segid 3A4 and resid 250 and name CB)	15.15	0.43	0.43
	assign (segid 3A4 and resid 241 and name CB)	(segid 3A4 and resid 251 and name CA)	16.57	0.15	0.15
	assign (segid 3A4 and resid 241 and name CB)	(segid 3A4 and resid 251 and name CB)	15.91	0.15	0.15
	assign (segid 3A4 and resid 241 and name CB)	(segid 3A4 and resid 252 and name CA)	17.57	0.23	0.24
	assign (segid 3A4 and resid 241 and name CB)	(segid 3A4 and resid 252 and name CB)	16.76	0.30	0.31
20	assign (segid 3A4 and resid 241 and name CB)	(segid 3A4 and resid 253 and name CA)	19.35	0.26	0.27
	assign (segid 3A4 and resid 241 and name N)	(segid 3A4 and resid 241 and name C)	2.48	0.01	0.01
	assign (segid 3A4 and resid 241 and name N)	(segid 3A4 and resid 241 and name CA)	1.46	0.02	0.02
	assign (segid 3A4 and resid 241 and name N)	(segid 3A4 and resid 241 and name CB)	2.44	0.03	0.02
	assign (segid 3A4 and resid 241 and name N)	(segid 3A4 and resid 241 and name O)	3.55	0.03	0.03
25	assign (segid 3A4 and resid 241 and name N)	(segid 3A4 and resid 242 and name C)	4.77	0.08	0.08
	assign (segid 3A4 and resid 241 and name N)	(segid 3A4 and resid 242 and name CA)	4.22	0.06	0.05
	assign (segid 3A4 and resid 241 and name N)	(segid 3A4 and resid 242 and name CB)	4.93	0.11	0.11
	assign (segid 3A4 and resid 241 and name N)	(segid 3A4 and resid 242 and name N)	2.80	0.04	0.04
	assign (segid 3A4 and resid 241 and name N)	(segid 3A4 and resid 242 and name O)	5.84	0.09	0.09
30	assign (segid 3A4 and resid 241 and name N)	(segid 3A4 and resid 243 and name C)	5.71	0.09	0.09
	assign (segid 3A4 and resid 241 and name N)	(segid 3A4 and resid 243 and name CA)	5.45	0.14	0.13
	assign (segid 3A4 and resid 241 and name N)	(segid 3A4 and resid 243 and name CB)	5.57	0.20	0.19
	assign (segid 3A4 and resid 241 and name N)	(segid 3A4 and resid 243 and name N)	4.42	0.11	0.11
	assign (segid 3A4 and resid 241 and name N)	(segid 3A4 and resid 243 and name O)	6.91	0.08	0.08
35	assign (segid 3A4 and resid 241 and name N)	(segid 3A4 and resid 244 and name C)	6.51	0.13	0.13
	assign (segid 3A4 and resid 241 and name N)	(segid 3A4 and resid 244 and name CA)	5.62	0.08	0.09
	assign (segid 3A4 and resid 241 and name N)	(segid 3A4 and resid 244 and name CB)	5.03	0.13	0.12
	assign (segid 3A4 and resid 241 and name N)	(segid 3A4 and resid 244 and name N)	4.87	0.07	0.07
	assign (segid 3A4 and resid 241 and name N)	(segid 3A4 and resid 244 and name O)	7.71	0.12	0.12
40	assign (segid 3A4 and resid 241 and name N)	(segid 3A4 and resid 245 and name CA)	7.30	0.21	0.21
	assign (segid 3A4 and resid 241 and name N)	(segid 3A4 and resid 245 and name CB)	7.09	0.24	0.25
	assign (segid 3A4 and resid 241 and name N)	(segid 3A4 and resid 245 and name N)	6.16	0.19	0.19
	assign (segid 3A4 and resid 241 and name N)	(segid 3A4 and resid 241 and name CB)	3.21	0.08	0.09
	assign (segid 3A4 and resid 241 and name O)	(segid 3A4 and resid 242 and name C)	3.07	0.16	0.17
45	assign (segid 3A4 and resid 241 and name O)	(segid 3A4 and resid 242 and name CA)	2.75	0.05	0.05
	assign (segid 3A4 and resid 241 and name O)	(segid 3A4 and resid 242 and name CB)	4.20	0.07	0.07
	assign (segid 3A4 and resid 241 and name O)	(segid 3A4 and resid 242 and name N)	2.24	0.01	0.01
	assign (segid 3A4 and resid 241 and name O)	(segid 3A4 and resid 242 and name O)	3.52	0.22	0.21
	assign (segid 3A4 and resid 241 and name O)	(segid 3A4 and resid 243 and name C)	4.29	0.28	0.27
50	assign (segid 3A4 and resid 241 and name O)	(segid 3A4 and resid 243 and name CA)	4.56	0.27	0.27
	assign (segid 3A4 and resid 241 and name O)	(segid 3A4 and resid 243 and name CB)	5.58	0.26	0.26
	assign (segid 3A4 and resid 241 and name O)	(segid 3A4 and resid 243 and name N)	3.59	0.23	0.22
	assign (segid 3A4 and resid 241 and name O)	(segid 3A4 and resid 243 and name O)	5.20	0.28	0.27
	assign (segid 3A4 and resid 241 and name O)	(segid 3A4 and resid 244 and name C)	3.99	0.26	0.27
55	assign (segid 3A4 and resid 241 and name O)	(segid 3A4 and resid 244 and name CA)	3.93	0.22	0.22
	assign (segid 3A4 and resid 241 and name O)	(segid 3A4 and resid 244 and name CB)	3.70	0.16	0.17
	assign (segid 3A4 and resid 241 and name O)	(segid 3A4 and resid 244 and name N)	3.51	0.26	0.25
	assign (segid 3A4 and resid 241 and name O)	(segid 3A4 and resid 244 and name O)	5.17	0.27	0.28
	assign (segid 3A4 and resid 241 and name O)	(segid 3A4 and resid 245 and name C)	5.14	0.32	0.33
60	assign (segid 3A4 and resid 241 and name O)	(segid 3A4 and resid 245 and name CA)	3.97	0.29	0.28
	assign (segid 3A4 and resid 241 and name O)	(segid 3A4 and resid 245 and name CB)	3.63	0.27	0.27
	assign (segid 3A4 and resid 241 and name O)	(segid 3A4 and resid 245 and name N)	3.13	0.27	0.28
	assign (segid 3A4 and resid 241 and name O)	(segid 3A4 and resid 245 and name O)	6.27	0.32	0.31
	assign (segid 3A4 and resid 241 and name O)	(segid 3A4 and resid 246 and name CA)	6.55	0.34	0.35
65	assign (segid 3A4 and resid 241 and name O)	(segid 3A4 and resid 246 and name CB)	6.79	0.34	0.35
	assign (segid 3A4 and resid 241 and name O)	(segid 3A4 and resid 246 and name N)	5.19	0.34	0.34
	assign (segid 3A4 and resid 241 and name O)	(segid 3A4 and resid 247 and name N)	7.13	0.31	0.30
	assign (segid 3A4 and resid 242 and name C)	(segid 3A4 and resid 242 and name CB)	2.51	0.02	0.01
	assign (segid 3A4 and resid 242 and name C)	(segid 3A4 and resid 242 and name O)	1.23	0.00	0.00
70	assign (segid 3A4 and resid 242 and name C)	(segid 3A4 and resid 243 and name C)	3.03	0.05	0.06
	assign (segid 3A4 and resid 242 and name C)	(segid 3A4 and resid 243 and name CA)	2.43	0.01	0.01
	assign (segid 3A4 and resid 242 and name C)	(segid 3A4 and resid 243 and name CB)	3.72	0.01	0.01
	assign (segid 3A4 and resid 242 and name C)	(segid 3A4 and resid 243 and name N)	1.33	0.01	0.00
	assign (segid 3A4 and resid 242 and name C)	(segid 3A4 and resid 243 and name O)	3.88	0.07	0.07
75	assign (segid 3A4 and resid 242 and name C)	(segid 3A4 and resid 244 and name C)	4.54	0.09	0.09
	assign (segid 3A4 and resid 242 and name C)	(segid 3A4 and resid 244 and name CA)	4.49	0.11	0.10
	assign (segid 3A4 and resid 242 and name C)	(segid 3A4 and resid 244 and name N)	3.30	0.10	0.11
	assign (segid 3A4 and resid 242 and name C)	(segid 3A4 and resid 244 and name O)	5.55	0.13	0.13
80	assign (segid 3A4 and resid 242 and name C)	(segid 3A4 and resid 245 and name C)	4.89	0.12	0.12
	assign (segid 3A4 and resid 242 and name C)	(segid 3A4 and resid 245 and name CA)	4.55	0.14	0.14
	assign (segid 3A4 and resid 242 and name C)	(segid 3A4 and resid 245 and name CB)	4.32	0.23	0.22
	assign (segid 3A4 and resid 242 and name C)	(segid 3A4 and resid 245 and name N)	3.85	0.12	0.12

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	assign (segid 3A4 and resid 242 and name C)	(segid 3A4 and resid 245 and name O)	6.11	0.12	0.12
	assign (segid 3A4 and resid 242 and name C)	(segid 3A4 and resid 246 and name C)	6.14	0.15	0.15
	assign (segid 3A4 and resid 242 and name C)	(segid 3A4 and resid 246 and name CA)	5.07	0.15	0.14
	assign (segid 3A4 and resid 242 and name C)	(segid 3A4 and resid 246 and name CB)	4.66	0.17	0.17
5	assign (segid 3A4 and resid 242 and name C)	(segid 3A4 and resid 246 and name N)	4.16	0.13	0.12
	assign (segid 3A4 and resid 242 and name C)	(segid 3A4 and resid 246 and name O)	7.29	0.15	0.14
	assign (segid 3A4 and resid 242 and name C)	(segid 3A4 and resid 247 and name CA)	7.32	0.16	0.15
	assign (segid 3A4 and resid 242 and name C)	(segid 3A4 and resid 247 and name CB)	7.41	0.19	0.18
	assign (segid 3A4 and resid 242 and name C)	(segid 3A4 and resid 247 and name N)	6.04	0.15	0.15
10	assign (segid 3A4 and resid 242 and name CA)	(segid 3A4 and resid 242 and name C)	1.53	0.01	0.01
	assign (segid 3A4 and resid 242 and name CA)	(segid 3A4 and resid 242 and name O)	1.52	0.01	0.02
	assign (segid 3A4 and resid 242 and name CA)	(segid 3A4 and resid 242 and name O)	2.40	0.01	0.01
	assign (segid 3A4 and resid 242 and name CA)	(segid 3A4 and resid 243 and name C)	4.41	0.05	0.06
	assign (segid 3A4 and resid 242 and name CA)	(segid 3A4 and resid 243 and name CA)	3.81	0.02	0.02
	assign (segid 3A4 and resid 242 and name CA)	(segid 3A4 and resid 243 and name CB)	4.88	0.03	0.03
15	assign (segid 3A4 and resid 242 and name CA)	(segid 3A4 and resid 243 and name N)	2.44	0.02	0.02
	assign (segid 3A4 and resid 242 and name CA)	(segid 3A4 and resid 243 and name O)	5.34	0.08	0.07
	assign (segid 3A4 and resid 242 and name CA)	(segid 3A4 and resid 244 and name C)	5.49	0.11	0.10
	assign (segid 3A4 and resid 242 and name CA)	(segid 3A4 and resid 244 and name CA)	5.43	0.13	0.14
20	assign (segid 3A4 and resid 242 and name CA)	(segid 3A4 and resid 244 and name CB)	5.78	0.23	0.22
	assign (segid 3A4 and resid 242 and name CA)	(segid 3A4 and resid 244 and name N)	4.37	0.10	0.11
	assign (segid 3A4 and resid 242 and name CA)	(segid 3A4 and resid 244 and name O)	6.58	0.12	0.13
	assign (segid 3A4 and resid 242 and name CA)	(segid 3A4 and resid 245 and name C)	5.77	0.14	0.14
	assign (segid 3A4 and resid 242 and name CA)	(segid 3A4 and resid 245 and name CA)	5.17	0.15	0.15
25	assign (segid 3A4 and resid 242 and name CA)	(segid 3A4 and resid 245 and name CB)	4.53	0.23	0.23
	assign (segid 3A4 and resid 242 and name CA)	(segid 3A4 and resid 245 and name N)	4.59	0.11	0.11
	assign (segid 3A4 and resid 242 and name CA)	(segid 3A4 and resid 245 and name O)	6.97	0.15	0.15
	assign (segid 3A4 and resid 242 and name CA)	(segid 3A4 and resid 246 and name C)	7.44	0.16	0.17
	assign (segid 3A4 and resid 242 and name CA)	(segid 3A4 and resid 246 and name CA)	6.26	0.18	0.18
30	assign (segid 3A4 and resid 242 and name CA)	(segid 3A4 and resid 246 and name CB)	5.92	0.21	0.22
	assign (segid 3A4 and resid 242 and name CA)	(segid 3A4 and resid 246 and name N)	5.25	0.15	0.15
	assign (segid 3A4 and resid 242 and name CA)	(segid 3A4 and resid 247 and name CA)	8.71	0.14	0.15
	assign (segid 3A4 and resid 242 and name CA)	(segid 3A4 and resid 247 and name CB)	8.81	0.18	0.18
	assign (segid 3A4 and resid 242 and name CA)	(segid 3A4 and resid 247 and name N)	7.42	0.15	0.15
35	assign (segid 3A4 and resid 242 and name CA)	(segid 3A4 and resid 248 and name CA)	10.01	0.15	0.14
	assign (segid 3A4 and resid 242 and name CA)	(segid 3A4 and resid 248 and name CB)	9.59	0.21	0.21
	assign (segid 3A4 and resid 242 and name CA)	(segid 3A4 and resid 249 and name CA)	10.63	0.15	0.16
	assign (segid 3A4 and resid 242 and name CA)	(segid 3A4 and resid 250 and name CA)	12.38	0.23	0.23
40	assign (segid 3A4 and resid 242 and name CA)	(segid 3A4 and resid 250 and name CB)	12.00	0.31	0.31
	assign (segid 3A4 and resid 242 and name CA)	(segid 3A4 and resid 251 and name CA)	14.38	0.16	0.16
	assign (segid 3A4 and resid 242 and name CA)	(segid 3A4 and resid 251 and name CB)	14.06	0.22	0.23
	assign (segid 3A4 and resid 242 and name CA)	(segid 3A4 and resid 252 and name CA)	15.57	0.20	0.20
	assign (segid 3A4 and resid 242 and name CA)	(segid 3A4 and resid 252 and name CB)	14.87	0.26	0.25
45	assign (segid 3A4 and resid 242 and name CA)	(segid 3A4 and resid 253 and name CA)	16.62	0.19	0.18
	assign (segid 3A4 and resid 242 and name CA)	(segid 3A4 and resid 254 and name CA)	18.05	0.34	0.33
	assign (segid 3A4 and resid 242 and name CA)	(segid 3A4 and resid 392 and name CB)	18.84	0.42	0.43
	assign (segid 3A4 and resid 242 and name CB)	(segid 3A4 and resid 243 and name C)	5.45	0.05	0.05
	assign (segid 3A4 and resid 242 and name CB)	(segid 3A4 and resid 243 and name CA)	4.50	0.04	0.04
	assign (segid 3A4 and resid 242 and name CB)	(segid 3A4 and resid 243 and name CB)	5.36	0.05	0.06
50	assign (segid 3A4 and resid 242 and name CB)	(segid 3A4 and resid 243 and name N)	3.17	0.05	0.05
	assign (segid 3A4 and resid 242 and name CB)	(segid 3A4 and resid 243 and name O)	6.34	0.08	0.07
	assign (segid 3A4 and resid 242 and name CB)	(segid 3A4 and resid 244 and name C)	6.90	0.10	0.10
	assign (segid 3A4 and resid 242 and name CB)	(segid 3A4 and resid 244 and name CA)	6.80	0.11	0.11
	assign (segid 3A4 and resid 242 and name CB)	(segid 3A4 and resid 244 and name CB)	7.20	0.19	0.19
55	assign (segid 3A4 and resid 242 and name CB)	(segid 3A4 and resid 244 and name N)	5.61	0.08	0.08
	assign (segid 3A4 and resid 242 and name CB)	(segid 3A4 and resid 245 and name C)	6.94	0.14	0.13
	assign (segid 3A4 and resid 242 and name CB)	(segid 3A4 and resid 245 and name CA)	6.50	0.15	0.16
	assign (segid 3A4 and resid 242 and name CB)	(segid 3A4 and resid 245 and name CB)	5.77	0.26	0.26
	assign (segid 3A4 and resid 242 and name CB)	(segid 3A4 and resid 245 and name N)	6.03	0.12	0.11
60	assign (segid 3A4 and resid 242 and name CB)	(segid 3A4 and resid 246 and name CA)	7.05	0.18	0.18
	assign (segid 3A4 and resid 242 and name CB)	(segid 3A4 and resid 246 and name CB)	6.45	0.22	0.22
	assign (segid 3A4 and resid 242 and name CB)	(segid 3A4 and resid 246 and name N)	6.26	0.14	0.14
	assign (segid 3A4 and resid 242 and name CB)	(segid 3A4 and resid 247 and name CA)	9.73	0.17	0.18
	assign (segid 3A4 and resid 242 and name CB)	(segid 3A4 and resid 247 and name CB)	9.88	0.21	0.22
65	assign (segid 3A4 and resid 242 and name CB)	(segid 3A4 and resid 248 and name CA)	11.28	0.15	0.15
	assign (segid 3A4 and resid 242 and name CB)	(segid 3A4 and resid 248 and name CB)	10.94	0.22	0.22
	assign (segid 3A4 and resid 242 and name CB)	(segid 3A4 and resid 249 and name CA)	11.61	0.16	0.17
	assign (segid 3A4 and resid 242 and name CB)	(segid 3A4 and resid 250 and name CA)	13.20	0.29	0.29
	assign (segid 3A4 and resid 242 and name CB)	(segid 3A4 and resid 250 and name CB)	12.75	0.36	0.36
70	assign (segid 3A4 and resid 242 and name CB)	(segid 3A4 and resid 251 and name CA)	15.45	0.20	0.20
	assign (segid 3A4 and resid 242 and name CB)	(segid 3A4 and resid 251 and name CB)	15.22	0.24	0.25
	assign (segid 3A4 and resid 242 and name CB)	(segid 3A4 and resid 252 and name CA)	16.66	0.22	0.21
	assign (segid 3A4 and resid 242 and name CB)	(segid 3A4 and resid 252 and name CB)	15.97	0.26	0.25
	assign (segid 3A4 and resid 242 and name CB)	(segid 3A4 and resid 253 and name CA)	17.45	0.27	0.28
75	assign (segid 3A4 and resid 242 and name CB)	(segid 3A4 and resid 254 and name CA)	18.85	0.45	0.44
	assign (segid 3A4 and resid 242 and name N)	(segid 3A4 and resid 242 and name C)	2.47	0.02	0.02
	assign (segid 3A4 and resid 242 and name N)	(segid 3A4 and resid 242 and name CA)	1.46	0.01	0.00
	assign (segid 3A4 and resid 242 and name N)	(segid 3A4 and resid 242 and name CB)	2.43	0.03	0.03
	assign (segid 3A4 and resid 242 and name N)	(segid 3A4 and resid 242 and name O)	3.50	0.04	0.03
80	assign (segid 3A4 and resid 242 and name N)	(segid 3A4 and resid 243 and name C)	4.68	0.02	0.03
	assign (segid 3A4 and resid 242 and name N)	(segid 3A4 and resid 243 and name CA)	4.22	0.04	0.03
	assign (segid 3A4 and resid 242 and name N)	(segid 3A4 and resid 243 and name CB)	4.99	0.06	0.06
	assign (segid 3A4 and resid 242 and name N)	(segid 3A4 and resid 243 and name N)	2.82	0.05	0.04

	assign (segid 3A4 and resid 242 and name N) (segid 3A4 and resid 243 and name O)	5.78	0.05	0.04
	assign (segid 3A4 and resid 242 and name N) (segid 3A4 and resid 244 and name C)	5.60	0.08	0.09
	assign (segid 3A4 and resid 242 and name N) (segid 3A4 and resid 244 and name CA)	5.27	0.11	0.11
	assign (segid 3A4 and resid 242 and name N) (segid 3A4 and resid 244 and name CB)	5.25	0.18	0.19
5	assign (segid 3A4 and resid 242 and name N) (segid 3A4 and resid 244 and name N)	4.27	0.07	0.08
	assign (segid 3A4 and resid 242 and name N) (segid 3A4 and resid 244 and name O)	6.79	0.08	0.09
	assign (segid 3A4 and resid 242 and name N) (segid 3A4 and resid 245 and name C)	6.51	0.17	0.17
	assign (segid 3A4 and resid 242 and name N) (segid 3A4 and resid 245 and name CA)	5.65	0.18	0.17
	assign (segid 3A4 and resid 242 and name N) (segid 3A4 and resid 245 and name CB)	5.12	0.23	0.23
10	assign (segid 3A4 and resid 242 and name N) (segid 3A4 and resid 245 and name N)	4.84	0.13	0.13
	assign (segid 3A4 and resid 242 and name N) (segid 3A4 and resid 246 and name CA)	7.29	0.17	0.17
	assign (segid 3A4 and resid 242 and name N) (segid 3A4 and resid 246 and name CB)	7.06	0.18	0.18
	assign (segid 3A4 and resid 242 and name N) (segid 3A4 and resid 246 and name N)	6.15	0.16	0.17
	assign (segid 3A4 and resid 242 and name N) (segid 3A4 and resid 242 and name CB)	3.31	0.06	0.06
15	assign (segid 3A4 and resid 242 and name O) (segid 3A4 and resid 243 and name C)	3.01	0.07	0.08
	assign (segid 3A4 and resid 242 and name O) (segid 3A4 and resid 243 and name CA)	2.77	0.05	0.04
	assign (segid 3A4 and resid 242 and name O) (segid 3A4 and resid 243 and name CB)	4.26	0.04	0.03
	assign (segid 3A4 and resid 242 and name O) (segid 3A4 and resid 243 and name N)	2.24	0.01	0.02
	assign (segid 3A4 and resid 242 and name O) (segid 3A4 and resid 244 and name C)	3.50	0.10	0.11
20	assign (segid 3A4 and resid 242 and name O) (segid 3A4 and resid 244 and name CA)	4.13	0.09	0.09
	assign (segid 3A4 and resid 242 and name O) (segid 3A4 and resid 244 and name CB)	4.45	0.10	0.11
	assign (segid 3A4 and resid 242 and name O) (segid 3A4 and resid 244 and name N)	5.35	0.16	0.17
	assign (segid 3A4 and resid 242 and name O) (segid 3A4 and resid 244 and name O)	3.49	0.10	0.11
	assign (segid 3A4 and resid 242 and name O) (segid 3A4 and resid 244 and name O)	4.97	0.14	0.14
25	assign (segid 3A4 and resid 242 and name O) (segid 3A4 and resid 245 and name C)	3.85	0.13	0.13
	assign (segid 3A4 and resid 242 and name O) (segid 3A4 and resid 245 and name CA)	3.76	0.15	0.16
	assign (segid 3A4 and resid 242 and name O) (segid 3A4 and resid 245 and name CB)	3.59	0.25	0.24
	assign (segid 3A4 and resid 242 and name O) (segid 3A4 and resid 245 and name N)	3.35	0.13	0.13
	assign (segid 3A4 and resid 242 and name O) (segid 3A4 and resid 245 and name O)	5.04	0.14	0.13
30	assign (segid 3A4 and resid 242 and name O) (segid 3A4 and resid 246 and name C)	5.08	0.17	0.17
	assign (segid 3A4 and resid 242 and name O) (segid 3A4 and resid 246 and name CA)	3.91	0.16	0.16
	assign (segid 3A4 and resid 242 and name O) (segid 3A4 and resid 246 and name CB)	3.61	0.19	0.19
	assign (segid 3A4 and resid 242 and name O) (segid 3A4 and resid 246 and name N)	3.03	0.14	0.13
	assign (segid 3A4 and resid 242 and name O) (segid 3A4 and resid 246 and name O)	6.19	0.16	0.16
35	assign (segid 3A4 and resid 242 and name O) (segid 3A4 and resid 247 and name C)	7.33	0.17	0.17
	assign (segid 3A4 and resid 242 and name O) (segid 3A4 and resid 247 and name CA)	6.50	0.18	0.19
	assign (segid 3A4 and resid 242 and name O) (segid 3A4 and resid 247 and name CB)	6.80	0.22	0.22
	assign (segid 3A4 and resid 242 and name O) (segid 3A4 and resid 247 and name N)	5.14	0.18	0.19
	assign (segid 3A4 and resid 242 and name O) (segid 3A4 and resid 248 and name N)	7.01	0.16	0.17
40	assign (segid 3A4 and resid 243 and name C) (segid 3A4 and resid 243 and name CB)	2.48	0.01	0.02
	assign (segid 3A4 and resid 243 and name C) (segid 3A4 and resid 243 and name O)	1.23	0.01	0.01
	assign (segid 3A4 and resid 243 and name C) (segid 3A4 and resid 244 and name C)	2.94	0.04	0.04
	assign (segid 3A4 and resid 243 and name C) (segid 3A4 and resid 244 and name CA)	2.43	0.02	0.02
	assign (segid 3A4 and resid 243 and name C) (segid 3A4 and resid 244 and name CB)	3.71	0.01	0.01
45	assign (segid 3A4 and resid 243 and name C) (segid 3A4 and resid 244 and name N)	1.33	0.01	0.00
	assign (segid 3A4 and resid 243 and name C) (segid 3A4 and resid 244 and name O)	3.69	0.15	0.14
	assign (segid 3A4 and resid 243 and name C) (segid 3A4 and resid 245 and name C)	4.49	0.10	0.09
	assign (segid 3A4 and resid 243 and name C) (segid 3A4 and resid 245 and name CA)	4.41	0.08	0.08
	assign (segid 3A4 and resid 243 and name C) (segid 3A4 and resid 245 and name CB)	5.15	0.13	0.13
50	assign (segid 3A4 and resid 243 and name C) (segid 3A4 and resid 245 and name N)	3.26	0.08	0.09
	assign (segid 3A4 and resid 243 and name C) (segid 3A4 and resid 245 and name O)	5.54	0.08	0.08
	assign (segid 3A4 and resid 243 and name C) (segid 3A4 and resid 246 and name CA)	4.83	0.11	0.10
	assign (segid 3A4 and resid 243 and name C) (segid 3A4 and resid 246 and name CB)	4.36	0.13	0.12
	assign (segid 3A4 and resid 243 and name C) (segid 3A4 and resid 246 and name N)	3.78	0.11	0.11
55	assign (segid 3A4 and resid 243 and name C) (segid 3A4 and resid 246 and name O)	6.02	0.10	0.10
	assign (segid 3A4 and resid 243 and name C) (segid 3A4 and resid 247 and name C)	6.12	0.13	0.13
	assign (segid 3A4 and resid 243 and name C) (segid 3A4 and resid 247 and name CA)	5.05	0.11	0.11
	assign (segid 3A4 and resid 243 and name C) (segid 3A4 and resid 247 and name CB)	4.71	0.16	0.16
60	assign (segid 3A4 and resid 243 and name C) (segid 3A4 and resid 247 and name N)	4.13	0.10	0.10
	assign (segid 3A4 and resid 243 and name C) (segid 3A4 and resid 247 and name O)	7.29	0.13	0.12
	assign (segid 3A4 and resid 243 and name C) (segid 3A4 and resid 248 and name CA)	7.25	0.19	0.18
	assign (segid 3A4 and resid 243 and name C) (segid 3A4 and resid 248 and name CB)	7.27	0.24	0.25
	assign (segid 3A4 and resid 243 and name C) (segid 3A4 and resid 248 and name N)	5.97	0.17	0.16
65	assign (segid 3A4 and resid 243 and name C) (segid 3A4 and resid 249 and name N)	7.75	0.12	0.11
	assign (segid 3A4 and resid 243 and name CA) (segid 3A4 and resid 243 and name C)	1.52	0.02	0.01
	assign (segid 3A4 and resid 243 and name CA) (segid 3A4 and resid 243 and name CB)	1.53	0.01	0.01
	assign (segid 3A4 and resid 243 and name CA) (segid 3A4 and resid 243 and name O)	2.38	0.02	0.02
	assign (segid 3A4 and resid 243 and name CA) (segid 3A4 and resid 244 and name C)	4.34	0.04	0.04
70	assign (segid 3A4 and resid 243 and name CA) (segid 3A4 and resid 244 and name CA)	3.81	0.01	0.00
	assign (segid 3A4 and resid 243 and name CA) (segid 3A4 and resid 244 and name CB)	4.86	0.03	0.03
	assign (segid 3A4 and resid 243 and name CA) (segid 3A4 and resid 244 and name N)	2.44	0.02	0.01
	assign (segid 3A4 and resid 243 and name CA) (segid 3A4 and resid 244 and name O)	5.14	0.14	0.15
	assign (segid 3A4 and resid 243 and name CA) (segid 3A4 and resid 245 and name C)	5.42	0.11	0.11
75	assign (segid 3A4 and resid 243 and name CA) (segid 3A4 and resid 245 and name CA)	5.39	0.11	0.11
	assign (segid 3A4 and resid 243 and name CA) (segid 3A4 and resid 245 and name CB)	5.80	0.18	0.17
	assign (segid 3A4 and resid 243 and name CA) (segid 3A4 and resid 245 and name N)	4.36	0.11	0.11
	assign (segid 3A4 and resid 243 and name CA) (segid 3A4 and resid 245 and name O)	6.54	0.11	0.10
	assign (segid 3A4 and resid 243 and name CA) (segid 3A4 and resid 246 and name C)	5.62	0.11	0.10
80	assign (segid 3A4 and resid 243 and name CA) (segid 3A4 and resid 246 and name CA)	5.05	0.11	0.11
	assign (segid 3A4 and resid 243 and name CA) (segid 3A4 and resid 246 and name CB)	4.46	0.13	0.13
	assign (segid 3A4 and resid 243 and name CA) (segid 3A4 and resid 246 and name N)	4.49	0.12	0.12
	assign (segid 3A4 and resid 243 and name CA) (segid 3A4 and resid 246 and name O)	6.76	0.09	0.10

	assign (segid 3A4 and resid 243 and name CA)	(segid 3A4 and resid 217 and name C)	7.34	0.15	0.16
	assign (segid 3A4 and resid 243 and name CA)	(segid 3A4 and resid 247 and name CA)	6.16	0.15	0.15
	assign (segid 3A4 and resid 243 and name CA)	(segid 3A4 and resid 247 and name CB)	5.92	0.21	0.21
	assign (segid 3A4 and resid 243 and name CA)	(segid 3A4 and resid 247 and name N)	5.15	0.14	0.14
	assign (segid 3A4 and resid 243 and name CA)	(segid 3A4 and resid 248 and name CA)	8.61	0.17	0.17
5	assign (segid 3A4 and resid 243 and name CA)	(segid 3A4 and resid 248 and name CB)	8.66	0.22	0.23
	assign (segid 3A4 and resid 243 and name CA)	(segid 3A4 and resid 248 and name N)	7.30	0.17	0.16
	assign (segid 3A4 and resid 243 and name CA)	(segid 3A4 and resid 249 and name CA)	9.79	0.09	0.10
	assign (segid 3A4 and resid 243 and name CA)	(segid 3A4 and resid 250 and name CA)	10.49	0.29	0.29
	assign (segid 3A4 and resid 243 and name CA)	(segid 3A4 and resid 250 and name CB)	9.75	0.38	0.39
10	assign (segid 3A4 and resid 243 and name CA)	(segid 3A4 and resid 251 and name CA)	12.28	0.18	0.19
	assign (segid 3A4 and resid 243 and name CA)	(segid 3A4 and resid 251 and name CB)	11.92	0.21	0.21
	assign (segid 3A4 and resid 243 and name CA)	(segid 3A4 and resid 252 and name CA)	14.29	0.11	0.12
	assign (segid 3A4 and resid 243 and name CA)	(segid 3A4 and resid 252 and name CB)	13.94	0.11	0.10
	assign (segid 3A4 and resid 243 and name CA)	(segid 3A4 and resid 253 and name CA)	15.36	0.23	0.23
15	assign (segid 3A4 and resid 243 and name CA)	(segid 3A4 and resid 254 and name CA)	16.05	0.40	0.40
	assign (segid 3A4 and resid 243 and name CA)	(segid 3A4 and resid 255 and name CA)	17.86	0.57	0.58
	assign (segid 3A4 and resid 243 and name CA)	(segid 3A4 and resid 389 and name CA)	17.69	0.71	0.72
	assign (segid 3A4 and resid 243 and name CA)	(segid 3A4 and resid 389 and name CB)	17.60	0.82	0.82
20	assign (segid 3A4 and resid 243 and name CA)	(segid 3A4 and resid 391 and name CA)	18.86	0.49	0.50
	assign (segid 3A4 and resid 243 and name CA)	(segid 3A4 and resid 392 and name CA)	17.01	0.49	0.48
	assign (segid 3A4 and resid 243 and name CA)	(segid 3A4 and resid 392 and name CB)	15.49	0.48	0.49
	assign (segid 3A4 and resid 243 and name CA)	(segid 3A4 and resid 393 and name CA)	18.51	0.52	0.51
	assign (segid 3A4 and resid 243 and name CA)	(segid 3A4 and resid 244 and name C)	5.35	0.03	0.04
	assign (segid 3A4 and resid 243 and name CB)	(segid 3A4 and resid 244 and name CA)	4.46	0.02	0.03
25	assign (segid 3A4 and resid 243 and name CB)	(segid 3A4 and resid 244 and name CB)	5.37	0.07	0.06
	assign (segid 3A4 and resid 243 and name CB)	(segid 3A4 and resid 244 and name N)	3.15	0.03	0.03
	assign (segid 3A4 and resid 243 and name CB)	(segid 3A4 and resid 244 and name O)	6.10	0.14	0.15
	assign (segid 3A4 and resid 243 and name CB)	(segid 3A4 and resid 245 and name C)	6.81	0.11	0.12
	assign (segid 3A4 and resid 243 and name CB)	(segid 3A4 and resid 245 and name CA)	6.76	0.11	0.11
30	assign (segid 3A4 and resid 243 and name CB)	(segid 3A4 and resid 245 and name CB)	7.24	0.17	0.18
	assign (segid 3A4 and resid 243 and name CB)	(segid 3A4 and resid 245 and name N)	5.60	0.11	0.11
	assign (segid 3A4 and resid 243 and name CB)	(segid 3A4 and resid 246 and name C)	6.71	0.13	0.13
	assign (segid 3A4 and resid 243 and name CB)	(segid 3A4 and resid 246 and name CA)	6.35	0.14	0.14
	assign (segid 3A4 and resid 243 and name CB)	(segid 3A4 and resid 246 and name CB)	5.67	0.19	0.18
35	assign (segid 3A4 and resid 243 and name CB)	(segid 3A4 and resid 246 and name N)	5.91	0.13	0.13
	assign (segid 3A4 and resid 243 and name CB)	(segid 3A4 and resid 246 and name O)	7.81	0.14	0.14
	assign (segid 3A4 and resid 243 and name CB)	(segid 3A4 and resid 247 and name CA)	6.86	0.14	0.15
	assign (segid 3A4 and resid 243 and name CB)	(segid 3A4 and resid 247 and name CB)	6.36	0.19	0.19
40	assign (segid 3A4 and resid 243 and name CB)	(segid 3A4 and resid 247 and name N)	6.09	0.14	0.14
	assign (segid 3A4 and resid 243 and name CB)	(segid 3A4 and resid 248 and name CA)	9.58	0.18	0.18
	assign (segid 3A4 and resid 243 and name CB)	(segid 3A4 and resid 248 and name CB)	9.70	0.24	0.25
	assign (segid 3A4 and resid 243 and name CB)	(segid 3A4 and resid 249 and name CA)	11.02	0.10	0.09
	assign (segid 3A4 and resid 243 and name CB)	(segid 3A4 and resid 250 and name CA)	11.37	0.32	0.33
	assign (segid 3A4 and resid 243 and name CB)	(segid 3A4 and resid 250 and name CB)	10.50	0.43	0.42
45	assign (segid 3A4 and resid 243 and name CB)	(segid 3A4 and resid 251 and name CA)	13.00	0.20	0.19
	assign (segid 3A4 and resid 243 and name CB)	(segid 3A4 and resid 251 and name CB)	12.57	0.21	0.22
	assign (segid 3A4 and resid 243 and name CB)	(segid 3A4 and resid 252 and name CA)	15.29	0.12	0.12
	assign (segid 3A4 and resid 243 and name CB)	(segid 3A4 and resid 252 and name CB)	15.03	0.09	0.09
	assign (segid 3A4 and resid 243 and name CB)	(segid 3A4 and resid 253 and name CA)	16.39	0.26	0.26
50	assign (segid 3A4 and resid 243 and name CB)	(segid 3A4 and resid 254 and name CA)	16.79	0.43	0.43
	assign (segid 3A4 and resid 243 and name CB)	(segid 3A4 and resid 255 and name CA)	18.58	0.62	0.61
	assign (segid 3A4 and resid 243 and name CB)	(segid 3A4 and resid 389 and name CA)	17.38	0.74	0.73
	assign (segid 3A4 and resid 243 and name CB)	(segid 3A4 and resid 389 and name CB)	17.34	0.80	0.79
	assign (segid 3A4 and resid 243 and name CB)	(segid 3A4 and resid 392 and name CA)	16.91	0.56	0.55
55	assign (segid 3A4 and resid 243 and name CB)	(segid 3A4 and resid 392 and name CB)	15.38	0.55	0.55
	assign (segid 3A4 and resid 243 and name CB)	(segid 3A4 and resid 393 and name CA)	18.65	0.59	0.59
	assign (segid 3A4 and resid 243 and name N)	(segid 3A4 and resid 243 and name C)	2.43	0.02	0.03
	assign (segid 3A4 and resid 243 and name N)	(segid 3A4 and resid 243 and name CA)	1.45	0.01	0.01
60	assign (segid 3A4 and resid 243 and name N)	(segid 3A4 and resid 243 and name CB)	2.47	0.02	0.01
	assign (segid 3A4 and resid 243 and name N)	(segid 3A4 and resid 243 and name O)	3.48	0.03	0.02
	assign (segid 3A4 and resid 243 and name N)	(segid 3A4 and resid 244 and name C)	4.64	0.04	0.04
	assign (segid 3A4 and resid 243 and name N)	(segid 3A4 and resid 244 and name CA)	4.18	0.06	0.05
	assign (segid 3A4 and resid 243 and name N)	(segid 3A4 and resid 244 and name CB)	4.90	0.10	0.11
65	assign (segid 3A4 and resid 243 and name N)	(segid 3A4 and resid 244 and name N)	2.78	0.06	0.05
	assign (segid 3A4 and resid 243 and name N)	(segid 3A4 and resid 244 and name O)	5.64	0.11	0.11
	assign (segid 3A4 and resid 243 and name N)	(segid 3A4 and resid 245 and name C)	5.58	0.10	0.10
	assign (segid 3A4 and resid 243 and name N)	(segid 3A4 and resid 245 and name CA)	5.28	0.12	0.11
	assign (segid 3A4 and resid 243 and name N)	(segid 3A4 and resid 245 and name CB)	5.33	0.18	0.18
70	assign (segid 3A4 and resid 243 and name N)	(segid 3A4 and resid 245 and name N)	4.29	0.10	0.11
	assign (segid 3A4 and resid 243 and name N)	(segid 3A4 and resid 245 and name O)	6.79	0.09	0.09
	assign (segid 3A4 and resid 243 and name N)	(segid 3A4 and resid 246 and name C)	6.42	0.11	0.11
	assign (segid 3A4 and resid 243 and name N)	(segid 3A4 and resid 246 and name CA)	5.58	0.11	0.10
	assign (segid 3A4 and resid 243 and name N)	(segid 3A4 and resid 246 and name CB)	5.05	0.10	0.10
75	assign (segid 3A4 and resid 243 and name N)	(segid 3A4 and resid 246 and name N)	4.78	0.10	0.11
	assign (segid 3A4 and resid 243 and name N)	(segid 3A4 and resid 246 and name O)	7.59	0.10	0.10
	assign (segid 3A4 and resid 243 and name N)	(segid 3A4 and resid 247 and name CA)	7.23	0.13	0.14
	assign (segid 3A4 and resid 243 and name N)	(segid 3A4 and resid 247 and name CB)	7.08	0.18	0.19
	assign (segid 3A4 and resid 243 and name N)	(segid 3A4 and resid 247 and name N)	6.10	0.13	0.13
80	assign (segid 3A4 and resid 243 and name N)	(segid 3A4 and resid 247 and name O)	3.24	0.05	0.06
	assign (segid 3A4 and resid 243 and name O)	(segid 3A4 and resid 243 and name CA)	2.90	0.10	0.10
	assign (segid 3A4 and resid 243 and name O)	(segid 3A4 and resid 244 and name C)	2.78	0.06	0.05
	assign (segid 3A4 and resid 243 and name O)	(segid 3A4 and resid 244 and name CA)	4.26	0.05	0.05
	assign (segid 3A4 and resid 243 and name O)	(segid 3A4 and resid 244 and name CB)			

	assign (segid 3A4 and resid 243 and name O)	(segid 3A4 and resid 244 and name N)	2.25	0.02	0.03
	assign (segid 3A4 and resid 243 and name O)	(segid 3A4 and resid 244 and name O)	3.23	0.22	0.23
	assign (segid 3A4 and resid 243 and name O)	(segid 3A4 and resid 245 and name C)	4.05	0.12	0.12
	assign (segid 3A4 and resid 243 and name O)	(segid 3A4 and resid 245 and name CA)	4.34	0.10	0.10
5	assign (segid 3A4 and resid 243 and name O)	(segid 3A4 and resid 245 and name CB)	5.30	0.12	0.13
	assign (segid 3A4 and resid 243 and name O)	(segid 3A4 and resid 245 and name N)	3.43	0.08	0.07
	assign (segid 3A4 and resid 243 and name O)	(segid 3A4 and resid 245 and name O)	4.94	0.12	0.12
	assign (segid 3A4 and resid 243 and name O)	(segid 3A4 and resid 246 and name C)	3.77	0.11	0.12
	assign (segid 3A4 and resid 243 and name O)	(segid 3A4 and resid 246 and name CA)	3.73	0.13	0.14
10	assign (segid 3A4 and resid 243 and name O)	(segid 3A4 and resid 246 and name CB)	3.70	0.17	0.17
	assign (segid 3A4 and resid 243 and name O)	(segid 3A4 and resid 246 and name N)	3.28	0.13	0.13
	assign (segid 3A4 and resid 243 and name O)	(segid 3A4 and resid 246 and name O)	4.93	0.11	0.11
	assign (segid 3A4 and resid 243 and name O)	(segid 3A4 and resid 247 and name C)	5.02	0.15	0.14
	assign (segid 3A4 and resid 243 and name O)	(segid 3A4 and resid 247 and name CA)	3.87	0.12	0.11
15	assign (segid 3A4 and resid 243 and name O)	(segid 3A4 and resid 247 and name CB)	3.63	0.17	0.18
	assign (segid 3A4 and resid 243 and name O)	(segid 3A4 and resid 247 and name N)	2.98	0.10	0.11
	assign (segid 3A4 and resid 243 and name O)	(segid 3A4 and resid 247 and name O)	6.15	0.14	0.14
	assign (segid 3A4 and resid 243 and name O)	(segid 3A4 and resid 248 and name C)	7.20	0.16	0.16
	assign (segid 3A4 and resid 243 and name O)	(segid 3A4 and resid 248 and name CA)	6.38	0.19	0.19
20	assign (segid 3A4 and resid 243 and name O)	(segid 3A4 and resid 248 and name CB)	6.62	0.24	0.24
	assign (segid 3A4 and resid 243 and name O)	(segid 3A4 and resid 248 and name N)	5.02	0.18	0.18
	assign (segid 3A4 and resid 243 and name O)	(segid 3A4 and resid 249 and name N)	6.83	0.11	0.11
	assign (segid 3A4 and resid 243 and name O)	(segid 3A4 and resid 250 and name N)	7.68	0.17	0.17
	assign (segid 3A4 and resid 243 and name O)	(segid 3A4 and resid 244 and name CB)	2.51	0.02	0.01
25	assign (segid 3A4 and resid 244 and name C)	(segid 3A4 and resid 244 and name O)	1.23	0.00	0.00
	assign (segid 3A4 and resid 244 and name C)	(segid 3A4 and resid 245 and name C)	3.02	0.05	0.04
	assign (segid 3A4 and resid 244 and name C)	(segid 3A4 and resid 245 and name CA)	2.44	0.01	0.01
	assign (segid 3A4 and resid 244 and name C)	(segid 3A4 and resid 245 and name CB)	3.72	0.03	0.03
	assign (segid 3A4 and resid 244 and name C)	(segid 3A4 and resid 245 and name N)	1.33	0.01	0.01
	assign (segid 3A4 and resid 244 and name C)	(segid 3A4 and resid 245 and name O)	3.83	0.05	0.06
30	assign (segid 3A4 and resid 244 and name C)	(segid 3A4 and resid 246 and name C)	4.58	0.08	0.09
	assign (segid 3A4 and resid 244 and name C)	(segid 3A4 and resid 246 and name CA)	4.47	0.08	0.09
	assign (segid 3A4 and resid 244 and name C)	(segid 3A4 and resid 246 and name CB)	5.25	0.10	0.10
	assign (segid 3A4 and resid 244 and name C)	(segid 3A4 and resid 246 and name N)	3.31	0.07	0.07
35	assign (segid 3A4 and resid 244 and name C)	(segid 3A4 and resid 246 and name O)	5.69	0.04	0.05
	assign (segid 3A4 and resid 244 and name C)	(segid 3A4 and resid 247 and name C)	4.93	0.07	0.07
	assign (segid 3A4 and resid 244 and name C)	(segid 3A4 and resid 247 and name CA)	4.59	0.13	0.14
	assign (segid 3A4 and resid 244 and name C)	(segid 3A4 and resid 247 and name CB)	4.41	0.21	0.21
	assign (segid 3A4 and resid 244 and name C)	(segid 3A4 and resid 247 and name N)	3.85	0.14	0.14
40	assign (segid 3A4 and resid 244 and name C)	(segid 3A4 and resid 247 and name O)	6.15	0.06	0.05
	assign (segid 3A4 and resid 244 and name C)	(segid 3A4 and resid 248 and name C)	6.14	0.15	0.15
	assign (segid 3A4 and resid 244 and name C)	(segid 3A4 and resid 248 and name CA)	5.10	0.14	0.14
	assign (segid 3A4 and resid 244 and name C)	(segid 3A4 and resid 248 and name CB)	4.70	0.25	0.24
	assign (segid 3A4 and resid 244 and name C)	(segid 3A4 and resid 248 and name N)	4.19	0.08	0.07
45	assign (segid 3A4 and resid 244 and name C)	(segid 3A4 and resid 248 and name O)	7.30	0.15	0.16
	assign (segid 3A4 and resid 244 and name C)	(segid 3A4 and resid 249 and name CA)	7.25	0.15	0.15
	assign (segid 3A4 and resid 244 and name C)	(segid 3A4 and resid 249 and name N)	5.99	0.15	0.14
	assign (segid 3A4 and resid 244 and name C)	(segid 3A4 and resid 250 and name N)	7.80	0.09	0.09
	assign (segid 3A4 and resid 244 and name CA)	(segid 3A4 and resid 244 and name C)	1.53	0.01	0.01
50	assign (segid 3A4 and resid 244 and name CA)	(segid 3A4 and resid 244 and name CB)	1.52	0.01	0.01
	assign (segid 3A4 and resid 244 and name CA)	(segid 3A4 and resid 244 and name O)	2.40	0.01	0.01
	assign (segid 3A4 and resid 244 and name CA)	(segid 3A4 and resid 245 and name C)	4.43	0.05	0.04
	assign (segid 3A4 and resid 244 and name CA)	(segid 3A4 and resid 245 and name CA)	3.82	0.02	0.02
	assign (segid 3A4 and resid 244 and name CA)	(segid 3A4 and resid 245 and name CB)	4.87	0.06	0.05
55	assign (segid 3A4 and resid 244 and name CA)	(segid 3A4 and resid 245 and name N)	2.44	0.04	0.03
	assign (segid 3A4 and resid 244 and name CA)	(segid 3A4 and resid 245 and name O)	5.31	0.06	0.06
	assign (segid 3A4 and resid 244 and name CA)	(segid 3A4 and resid 246 and name C)	5.57	0.09	0.09
	assign (segid 3A4 and resid 244 and name CA)	(segid 3A4 and resid 246 and name CA)	5.51	0.09	0.08
	assign (segid 3A4 and resid 244 and name CA)	(segid 3A4 and resid 246 and name CB)	5.97	0.09	0.09
60	assign (segid 3A4 and resid 244 and name CA)	(segid 3A4 and resid 246 and name N)	4.44	0.07	0.07
	assign (segid 3A4 and resid 244 and name CA)	(segid 3A4 and resid 246 and name O)	6.72	0.08	0.07
	assign (segid 3A4 and resid 244 and name CA)	(segid 3A4 and resid 247 and name C)	5.82	0.09	0.08
	assign (segid 3A4 and resid 244 and name CA)	(segid 3A4 and resid 247 and name CA)	5.23	0.10	0.11
	assign (segid 3A4 and resid 244 and name CA)	(segid 3A4 and resid 247 and name CB)	4.65	0.17	0.16
65	assign (segid 3A4 and resid 244 and name CA)	(segid 3A4 and resid 247 and name N)	4.65	0.10	0.09
	assign (segid 3A4 and resid 244 and name CA)	(segid 3A4 and resid 247 and name O)	7.02	0.09	0.10
	assign (segid 3A4 and resid 244 and name CA)	(segid 3A4 and resid 248 and name C)	7.42	0.17	0.16
	assign (segid 3A4 and resid 244 and name CA)	(segid 3A4 and resid 248 and name CA)	6.25	0.17	0.18
	assign (segid 3A4 and resid 244 and name CA)	(segid 3A4 and resid 248 and name CB)	5.92	0.27	0.28
70	assign (segid 3A4 and resid 244 and name CA)	(segid 3A4 and resid 248 and name N)	5.25	0.12	0.13
	assign (segid 3A4 and resid 244 and name CA)	(segid 3A4 and resid 249 and name CA)	8.65	0.15	0.14
	assign (segid 3A4 and resid 244 and name CA)	(segid 3A4 and resid 249 and name N)	7.36	0.15	0.15
	assign (segid 3A4 and resid 244 and name CA)	(segid 3A4 and resid 250 and name CA)	9.95	0.16	0.16
	assign (segid 3A4 and resid 244 and name CA)	(segid 3A4 and resid 250 and name CB)	9.55	0.28	0.28
75	assign (segid 3A4 and resid 244 and name CA)	(segid 3A4 and resid 251 and name CA)	10.68	0.14	0.14
	assign (segid 3A4 and resid 244 and name CA)	(segid 3A4 and resid 251 and name CB)	9.94	0.19	0.19
	assign (segid 3A4 and resid 244 and name CA)	(segid 3A4 and resid 252 and name CA)	12.48	0.20	0.21
	assign (segid 3A4 and resid 244 and name CA)	(segid 3A4 and resid 252 and name CB)	12.06	0.23	0.24
	assign (segid 3A4 and resid 244 and name CA)	(segid 3A4 and resid 253 and name CA)	14.41	0.10	0.10
80	assign (segid 3A4 and resid 244 and name CA)	(segid 3A4 and resid 254 and name CA)	15.29	0.14	0.13
	assign (segid 3A4 and resid 244 and name CA)	(segid 3A4 and resid 255 and name CA)	16.39	0.69	0.68
	assign (segid 3A4 and resid 244 and name CA)	(segid 3A4 and resid 256 and name CA)	18.38	0.38	0.38
	assign (segid 3A4 and resid 244 and name CA)	(segid 3A4 and resid 389 and name CA)	18.54	0.45	0.44

	assign (segid 3A4 and resid 244 and name CA)	(segid 3A4 and resid 389 and name CB)	18.66	0.57	0.57
	assign (segid 3A4 and resid 244 and name CA)	(segid 3A4 and resid 391 and name CA)	18.53	0.36	0.35
	assign (segid 3A4 and resid 244 and name CA)	(segid 3A4 and resid 392 and name CA)	16.19	0.40	0.40
	assign (segid 3A4 and resid 244 and name CA)	(segid 3A4 and resid 392 and name CB)	14.69	0.39	0.38
5	assign (segid 3A4 and resid 244 and name CA)	(segid 3A4 and resid 393 and name CA)	17.10	0.47	0.47
	assign (segid 3A4 and resid 244 and name CA)	(segid 3A4 and resid 396 and name CB)	18.83	0.65	0.65
	assign (segid 3A4 and resid 244 and name CA)	(segid 3A4 and resid 245 and name C)	5.40	0.08	0.08
	assign (segid 3A4 and resid 244 and name CB)	(segid 3A4 and resid 245 and name CA)	4.43	0.09	0.09
	assign (segid 3A4 and resid 244 and name CB)	(segid 3A4 and resid 245 and name CB)	5.28	0.09	0.10
	assign (segid 3A4 and resid 244 and name CB)	(segid 3A4 and resid 245 and name N)	3.10	0.11	0.10
10	assign (segid 3A4 and resid 244 and name CB)	(segid 3A4 and resid 245 and name O)	6.25	0.09	0.09
	assign (segid 3A4 and resid 244 and name CB)	(segid 3A4 and resid 246 and name C)	6.96	0.09	0.09
	assign (segid 3A4 and resid 244 and name CB)	(segid 3A4 and resid 246 and name CA)	6.83	0.07	0.07
	assign (segid 3A4 and resid 244 and name CB)	(segid 3A4 and resid 246 and name CB)	7.35	0.09	0.09
	assign (segid 3A4 and resid 244 and name CB)	(segid 3A4 and resid 246 and name N)	5.63	0.07	0.06
15	assign (segid 3A4 and resid 244 and name CB)	(segid 3A4 and resid 247 and name C)	6.98	0.09	0.09
	assign (segid 3A4 and resid 244 and name CB)	(segid 3A4 and resid 247 and name CA)	6.58	0.13	0.13
	assign (segid 3A4 and resid 244 and name CB)	(segid 3A4 and resid 247 and name CB)	5.92	0.18	0.17
	assign (segid 3A4 and resid 244 and name CB)	(segid 3A4 and resid 247 and name N)	6.07	0.11	0.11
	assign (segid 3A4 and resid 244 and name CB)	(segid 3A4 and resid 248 and name CA)	7.03	0.16	0.15
20	assign (segid 3A4 and resid 244 and name CB)	(segid 3A4 and resid 248 and name CB)	6.42	0.25	0.25
	assign (segid 3A4 and resid 244 and name CB)	(segid 3A4 and resid 248 and name N)	6.25	0.11	0.11
	assign (segid 3A4 and resid 244 and name CB)	(segid 3A4 and resid 249 and name CA)	9.64	0.16	0.15
	assign (segid 3A4 and resid 244 and name CB)	(segid 3A4 and resid 250 and name CA)	11.21	0.15	0.14
	assign (segid 3A4 and resid 244 and name CB)	(segid 3A4 and resid 250 and name CB)	10.90	0.28	0.27
25	assign (segid 3A4 and resid 244 and name CB)	(segid 3A4 and resid 251 and name CA)	11.66	0.17	0.17
	assign (segid 3A4 and resid 244 and name CB)	(segid 3A4 and resid 251 and name CB)	10.80	0.22	0.23
	assign (segid 3A4 and resid 244 and name CB)	(segid 3A4 and resid 252 and name CA)	13.29	0.26	0.26
	assign (segid 3A4 and resid 244 and name CB)	(segid 3A4 and resid 252 and name CB)	12.79	0.29	0.30
	assign (segid 3A4 and resid 244 and name CB)	(segid 3A4 and resid 253 and name CA)	15.46	0.15	0.14
30	assign (segid 3A4 and resid 244 and name CB)	(segid 3A4 and resid 254 and name CA)	16.44	0.09	0.10
	assign (segid 3A4 and resid 244 and name CB)	(segid 3A4 and resid 255 and name CA)	17.32	0.75	0.76
	assign (segid 3A4 and resid 244 and name CB)	(segid 3A4 and resid 256 and name CA)	19.22	0.47	0.47
	assign (segid 3A4 and resid 244 and name CB)	(segid 3A4 and resid 392 and name CA)	17.20	0.37	0.37
	assign (segid 3A4 and resid 244 and name CB)	(segid 3A4 and resid 392 and name CB)	15.71	0.36	0.35
35	assign (segid 3A4 and resid 244 and name CB)	(segid 3A4 and resid 393 and name CA)	18.00	0.47	0.46
	assign (segid 3A4 and resid 244 and name CB)	(segid 3A4 and resid 244 and name C)	2.42	0.02	0.02
	assign (segid 3A4 and resid 244 and name N)	(segid 3A4 and resid 244 and name CA)	1.46	0.01	0.00
	assign (segid 3A4 and resid 244 and name N)	(segid 3A4 and resid 244 and name CB)	2.45	0.02	0.02
	assign (segid 3A4 and resid 244 and name N)	(segid 3A4 and resid 244 and name O)	3.41	0.06	0.07
40	assign (segid 3A4 and resid 244 and name N)	(segid 3A4 and resid 245 and name C)	4.68	0.08	0.08
	assign (segid 3A4 and resid 244 and name N)	(segid 3A4 and resid 245 and name CA)	4.19	0.09	0.08
	assign (segid 3A4 and resid 244 and name N)	(segid 3A4 and resid 245 and name CB)	4.94	0.12	0.12
	assign (segid 3A4 and resid 244 and name N)	(segid 3A4 and resid 245 and name N)	2.80	0.08	0.09
	assign (segid 3A4 and resid 244 and name N)	(segid 3A4 and resid 245 and name O)	5.75	0.08	0.08
45	assign (segid 3A4 and resid 244 and name N)	(segid 3A4 and resid 246 and name C)	5.63	0.10	0.11
	assign (segid 3A4 and resid 244 and name N)	(segid 3A4 and resid 246 and name CA)	5.32	0.11	0.11
	assign (segid 3A4 and resid 244 and name N)	(segid 3A4 and resid 246 and name CB)	5.43	0.11	0.10
	assign (segid 3A4 and resid 244 and name N)	(segid 3A4 and resid 246 and name N)	4.32	0.10	0.10
	assign (segid 3A4 and resid 244 and name N)	(segid 3A4 and resid 246 and name O)	6.84	0.10	0.10
50	assign (segid 3A4 and resid 244 and name N)	(segid 3A4 and resid 247 and name C)	6.52	0.11	0.10
	assign (segid 3A4 and resid 244 and name N)	(segid 3A4 and resid 247 and name CA)	5.67	0.10	0.09
	assign (segid 3A4 and resid 244 and name N)	(segid 3A4 and resid 247 and name CB)	5.17	0.14	0.15
	assign (segid 3A4 and resid 244 and name N)	(segid 3A4 and resid 247 and name N)	4.86	0.09	0.09
	assign (segid 3A4 and resid 244 and name N)	(segid 3A4 and resid 247 and name O)	7.73	0.11	0.11
55	assign (segid 3A4 and resid 244 and name N)	(segid 3A4 and resid 248 and name CA)	7.27	0.18	0.18
	assign (segid 3A4 and resid 244 and name N)	(segid 3A4 and resid 248 and name CB)	7.05	0.26	0.27
	assign (segid 3A4 and resid 244 and name N)	(segid 3A4 and resid 248 and name N)	6.13	0.15	0.15
	assign (segid 3A4 and resid 244 and name N)	(segid 3A4 and resid 248 and name O)	3.37	0.07	0.06
	assign (segid 3A4 and resid 244 and name O)	(segid 3A4 and resid 245 and name C)	2.93	0.09	0.10
60	assign (segid 3A4 and resid 244 and name O)	(segid 3A4 and resid 245 and name CA)	2.79	0.04	0.03
	assign (segid 3A4 and resid 244 and name O)	(segid 3A4 and resid 245 and name CB)	4.27	0.03	0.03
	assign (segid 3A4 and resid 244 and name O)	(segid 3A4 and resid 245 and name N)	2.25	0.01	0.02
	assign (segid 3A4 and resid 244 and name O)	(segid 3A4 and resid 245 and name O)	3.39	0.10	0.10
	assign (segid 3A4 and resid 244 and name O)	(segid 3A4 and resid 246 and name C)	4.06	0.21	0.20
65	assign (segid 3A4 and resid 244 and name O)	(segid 3A4 and resid 246 and name CA)	4.30	0.19	0.20
	assign (segid 3A4 and resid 244 and name O)	(segid 3A4 and resid 246 and name CB)	5.29	0.23	0.24
	assign (segid 3A4 and resid 244 and name O)	(segid 3A4 and resid 246 and name N)	3.38	0.15	0.16
	assign (segid 3A4 and resid 244 and name O)	(segid 3A4 and resid 246 and name O)	5.03	0.15	0.15
	assign (segid 3A4 and resid 244 and name O)	(segid 3A4 and resid 247 and name C)	3.84	0.13	0.13
70	assign (segid 3A4 and resid 244 and name O)	(segid 3A4 and resid 247 and name CA)	3.73	0.27	0.27
	assign (segid 3A4 and resid 244 and name O)	(segid 3A4 and resid 247 and name CB)	3.62	0.34	0.35
	assign (segid 3A4 and resid 244 and name O)	(segid 3A4 and resid 247 and name N)	3.23	0.31	0.30
	assign (segid 3A4 and resid 244 and name O)	(segid 3A4 and resid 247 and name O)	5.03	0.10	0.11
	assign (segid 3A4 and resid 244 and name O)	(segid 3A4 and resid 248 and name C)	5.06	0.17	0.17
75	assign (segid 3A4 and resid 244 and name O)	(segid 3A4 and resid 248 and name CA)	3.95	0.18	0.19
	assign (segid 3A4 and resid 244 and name O)	(segid 3A4 and resid 248 and name CB)	3.69	0.33	0.34
	assign (segid 3A4 and resid 244 and name O)	(segid 3A4 and resid 248 and name N)	3.04	0.09	0.09
	assign (segid 3A4 and resid 244 and name O)	(segid 3A4 and resid 248 and name O)	6.21	0.18	0.17
	assign (segid 3A4 and resid 244 and name O)	(segid 3A4 and resid 249 and name C)	7.20	0.08	0.09
80	assign (segid 3A4 and resid 244 and name O)	(segid 3A4 and resid 249 and name CA)	6.38	0.14	0.14
	assign (segid 3A4 and resid 244 and name O)	(segid 3A4 and resid 249 and name N)	5.04	0.15	0.15
	assign (segid 3A4 and resid 244 and name O)	(segid 3A4 and resid 250 and name N)	6.85	0.10	0.10

	assign (segid 3A4 and resid 244 and name O) (segid 3A4 and resid 251 and name N)	7.76	0.10	0.11
	assign (segid 3A4 and resid 245 and name C) (segid 3A4 and resid 245 and name CB)	2.49	0.03	0.02
	assign (segid 3A4 and resid 245 and name C) (segid 3A4 and resid 245 and name O)	1.23	0.01	0.01
	assign (segid 3A4 and resid 245 and name C) (segid 3A4 and resid 246 and name C)	3.08	0.04	0.04
5	assign (segid 3A4 and resid 245 and name C) (segid 3A4 and resid 246 and name CA)	2.45	0.02	0.01
	assign (segid 3A4 and resid 245 and name C) (segid 3A4 and resid 246 and name CB)	3.72	0.02	0.01
	assign (segid 3A4 and resid 245 and name C) (segid 3A4 and resid 246 and name N)	1.33	0.01	0.00
	assign (segid 3A4 and resid 245 and name C) (segid 3A4 and resid 246 and name O)	3.96	0.05	0.06
	assign (segid 3A4 and resid 245 and name C) (segid 3A4 and resid 247 and name C)	4.54	0.12	0.11
	assign (segid 3A4 and resid 245 and name C) (segid 3A4 and resid 247 and name CA)	4.48	0.13	0.13
10	assign (segid 3A4 and resid 245 and name C) (segid 3A4 and resid 247 and name CB)	5.25	0.19	0.18
	assign (segid 3A4 and resid 245 and name C) (segid 3A4 and resid 247 and name N)	3.30	0.12	0.13
	assign (segid 3A4 and resid 245 and name C) (segid 3A4 and resid 247 and name O)	5.57	0.11	0.11
	assign (segid 3A4 and resid 245 and name C) (segid 3A4 and resid 248 and name C)	4.87	0.09	0.09
	assign (segid 3A4 and resid 245 and name C) (segid 3A4 and resid 248 and name CA)	4.58	0.07	0.06
15	assign (segid 3A4 and resid 245 and name C) (segid 3A4 and resid 248 and name CB)	4.38	0.12	0.11
	assign (segid 3A4 and resid 245 and name C) (segid 3A4 and resid 248 and name N)	3.86	0.09	0.08
	assign (segid 3A4 and resid 245 and name C) (segid 3A4 and resid 248 and name O)	6.07	0.10	0.11
	assign (segid 3A4 and resid 245 and name C) (segid 3A4 and resid 249 and name C)	6.09	0.09	0.09
	assign (segid 3A4 and resid 245 and name C) (segid 3A4 and resid 249 and name CA)	5.01	0.11	0.11
20	assign (segid 3A4 and resid 245 and name C) (segid 3A4 and resid 249 and name N)	4.14	0.09	0.08
	assign (segid 3A4 and resid 245 and name C) (segid 3A4 and resid 249 and name O)	7.25	0.10	0.09
	assign (segid 3A4 and resid 245 and name C) (segid 3A4 and resid 250 and name CA)	7.26	0.14	0.14
	assign (segid 3A4 and resid 245 and name C) (segid 3A4 and resid 250 and name CB)	7.31	0.22	0.21
	assign (segid 3A4 and resid 245 and name C) (segid 3A4 and resid 250 and name N)	5.97	0.11	0.12
25	assign (segid 3A4 and resid 245 and name CA) (segid 3A4 and resid 245 and name C)	1.52	0.01	0.01
	assign (segid 3A4 and resid 245 and name CA) (segid 3A4 and resid 245 and name CB)	1.53	0.01	0.02
	assign (segid 3A4 and resid 245 and name CA) (segid 3A4 and resid 245 and name O)	2.39	0.03	0.03
	assign (segid 3A4 and resid 245 and name CA) (segid 3A4 and resid 246 and name C)	4.46	0.03	0.03
30	assign (segid 3A4 and resid 245 and name CA) (segid 3A4 and resid 246 and name CA)	3.81	0.02	0.03
	assign (segid 3A4 and resid 245 and name CA) (segid 3A4 and resid 246 and name CB)	4.86	0.02	0.03
	assign (segid 3A4 and resid 245 and name CA) (segid 3A4 and resid 246 and name N)	2.44	0.02	0.02
	assign (segid 3A4 and resid 245 and name CA) (segid 3A4 and resid 246 and name O)	5.43	0.05	0.05
	assign (segid 3A4 and resid 245 and name CA) (segid 3A4 and resid 247 and name C)	5.50	0.12	0.13
35	assign (segid 3A4 and resid 245 and name CA) (segid 3A4 and resid 247 and name CA)	5.48	0.13	0.14
	assign (segid 3A4 and resid 245 and name CA) (segid 3A4 and resid 247 and name CB)	5.92	0.21	0.22
	assign (segid 3A4 and resid 245 and name CA) (segid 3A4 and resid 247 and name N)	4.41	0.12	0.12
	assign (segid 3A4 and resid 245 and name CA) (segid 3A4 and resid 247 and name O)	6.61	0.12	0.12
	assign (segid 3A4 and resid 245 and name CA) (segid 3A4 and resid 248 and name C)	5.72	0.09	0.09
40	assign (segid 3A4 and resid 245 and name CA) (segid 3A4 and resid 248 and name CA)	5.17	0.05	0.06
	assign (segid 3A4 and resid 245 and name CA) (segid 3A4 and resid 248 and name CB)	4.56	0.10	0.09
	assign (segid 3A4 and resid 245 and name CA) (segid 3A4 and resid 248 and name N)	4.60	0.09	0.10
	assign (segid 3A4 and resid 245 and name CA) (segid 3A4 and resid 248 and name O)	6.89	0.12	0.12
	assign (segid 3A4 and resid 245 and name CA) (segid 3A4 and resid 249 and name C)	7.37	0.09	0.08
45	assign (segid 3A4 and resid 245 and name CA) (segid 3A4 and resid 249 and name CA)	6.18	0.12	0.11
	assign (segid 3A4 and resid 245 and name CA) (segid 3A4 and resid 249 and name N)	5.20	0.08	0.09
	assign (segid 3A4 and resid 245 and name CA) (segid 3A4 and resid 250 and name CA)	8.64	0.14	0.13
	assign (segid 3A4 and resid 245 and name CA) (segid 3A4 and resid 250 and name CB)	8.71	0.22	0.22
	assign (segid 3A4 and resid 245 and name CA) (segid 3A4 and resid 250 and name N)	7.33	0.11	0.11
50	assign (segid 3A4 and resid 245 and name CA) (segid 3A4 and resid 251 and name CA)	9.99	0.13	0.13
	assign (segid 3A4 and resid 245 and name CA) (segid 3A4 and resid 251 and name CB)	9.60	0.17	0.16
	assign (segid 3A4 and resid 245 and name CA) (segid 3A4 and resid 252 and name CA)	10.74	0.21	0.22
	assign (segid 3A4 and resid 245 and name CA) (segid 3A4 and resid 252 and name CB)	9.96	0.25	0.26
	assign (segid 3A4 and resid 245 and name CA) (segid 3A4 and resid 253 and name CA)	12.37	0.22	0.21
55	assign (segid 3A4 and resid 245 and name CA) (segid 3A4 and resid 254 and name CA)	14.09	0.16	0.15
	assign (segid 3A4 and resid 245 and name CA) (segid 3A4 and resid 255 and name CA)	15.36	0.60	0.60
	assign (segid 3A4 and resid 245 and name CA) (segid 3A4 and resid 256 and name CA)	16.72	0.50	0.50
	assign (segid 3A4 and resid 245 and name CA) (segid 3A4 and resid 257 and name CA)	18.90	0.55	0.54
	assign (segid 3A4 and resid 245 and name CA) (segid 3A4 and resid 391 and name CA)	19.17	0.33	0.33
60	assign (segid 3A4 and resid 245 and name CA) (segid 3A4 and resid 392 and name CA)	17.32	0.43	0.44
	assign (segid 3A4 and resid 245 and name CA) (segid 3A4 and resid 392 and name CB)	15.91	0.45	0.44
	assign (segid 3A4 and resid 245 and name CA) (segid 3A4 and resid 393 and name CA)	17.71	0.47	0.47
	assign (segid 3A4 and resid 245 and name CB) (segid 3A4 and resid 246 and name C)	5.45	0.06	0.05
	assign (segid 3A4 and resid 245 and name CB) (segid 3A4 and resid 246 and name CA)	4.45	0.06	0.06
65	assign (segid 3A4 and resid 245 and name CB) (segid 3A4 and resid 246 and name CB)	5.27	0.08	0.09
	assign (segid 3A4 and resid 245 and name CB) (segid 3A4 and resid 246 and name N)	3.11	0.06	0.07
	assign (segid 3A4 and resid 245 and name CB) (segid 3A4 and resid 246 and name O)	6.36	0.05	0.05
	assign (segid 3A4 and resid 245 and name CB) (segid 3A4 and resid 247 and name C)	6.90	0.15	0.14
	assign (segid 3A4 and resid 245 and name CB) (segid 3A4 and resid 247 and name CA)	6.83	0.14	0.13
70	assign (segid 3A4 and resid 245 and name CB) (segid 3A4 and resid 247 and name CB)	7.34	0.20	0.20
	assign (segid 3A4 and resid 245 and name CB) (segid 3A4 and resid 247 and name N)	5.63	0.13	0.12
	assign (segid 3A4 and resid 245 and name CB) (segid 3A4 and resid 248 and name C)	6.87	0.11	0.11
	assign (segid 3A4 and resid 245 and name CB) (segid 3A4 and resid 248 and name CA)	6.51	0.10	0.11
	assign (segid 3A4 and resid 245 and name CB) (segid 3A4 and resid 248 and name CB)	5.82	0.12	0.11
75	assign (segid 3A4 and resid 245 and name CB) (segid 3A4 and resid 248 and name N)	6.04	0.14	0.13
	assign (segid 3A4 and resid 245 and name CB) (segid 3A4 and resid 249 and name CA)	6.94	0.10	0.10
	assign (segid 3A4 and resid 245 and name CB) (segid 3A4 and resid 249 and name N)	6.20	0.08	0.08
	assign (segid 3A4 and resid 245 and name CB) (segid 3A4 and resid 250 and name CA)	9.64	0.16	0.16
	assign (segid 3A4 and resid 245 and name CB) (segid 3A4 and resid 250 and name CB)	9.76	0.23	0.22
80	assign (segid 3A4 and resid 245 and name CB) (segid 3A4 and resid 251 and name CA)	11.25	0.13	0.14
	assign (segid 3A4 and resid 245 and name CB) (segid 3A4 and resid 251 and name CB)	10.95	0.16	0.16
	assign (segid 3A4 and resid 245 and name CB) (segid 3A4 and resid 252 and name CA)	11.71	0.22	0.21
	assign (segid 3A4 and resid 245 and name CB) (segid 3A4 and resid 252 and name CB)	10.80	0.25	0.25

	assign (segid 3A4 and resid 245 and name CB)	(segid 3A4 and resid 253 and name CA)	13.12	0.27	0.27
	assign (segid 3A4 and resid 245 and name CB)	(segid 3A4 and resid 254 and name CA)	15.08	0.22	0.21
	assign (segid 3A4 and resid 245 and name CB)	(segid 3A4 and resid 255 and name CA)	16.46	0.56	0.57
	assign (segid 3A4 and resid 245 and name CB)	(segid 3A4 and resid 256 and name CA)	17.62	0.53	0.54
	assign (segid 3A4 and resid 245 and name CB)	(segid 3A4 and resid 392 and name CA)	18.74	0.44	0.44
5	assign (segid 3A4 and resid 245 and name CB)	(segid 3A4 and resid 392 and name CB)	17.33	0.45	0.45
	assign (segid 3A4 and resid 245 and name CB)	(segid 3A4 and resid 393 and name CA)	19.12	0.48	0.48
	assign (segid 3A4 and resid 245 and name CB)	(segid 3A4 and resid 245 and name C)	2.46	0.02	0.02
	assign (segid 3A4 and resid 245 and name N)	(segid 3A4 and resid 245 and name CA)	1.46	0.01	0.00
	assign (segid 3A4 and resid 245 and name N)	(segid 3A4 and resid 245 and name CB)	2.46	0.02	0.03
10	assign (segid 3A4 and resid 245 and name N)	(segid 3A4 and resid 245 and name O)	3.48	0.02	0.02
	assign (segid 3A4 and resid 245 and name N)	(segid 3A4 and resid 246 and name C)	4.75	0.04	0.05
	assign (segid 3A4 and resid 245 and name N)	(segid 3A4 and resid 246 and name CA)	4.24	0.05	0.05
	assign (segid 3A4 and resid 245 and name N)	(segid 3A4 and resid 246 and name CB)	5.01	0.06	0.05
	assign (segid 3A4 and resid 245 and name N)	(segid 3A4 and resid 246 and name N)	2.84	0.05	0.05
15	assign (segid 3A4 and resid 245 and name N)	(segid 3A4 and resid 246 and name O)	5.88	0.06	0.05
	assign (segid 3A4 and resid 245 and name N)	(segid 3A4 and resid 247 and name C)	5.65	0.06	0.06
	assign (segid 3A4 and resid 245 and name N)	(segid 3A4 and resid 247 and name CA)	5.36	0.09	0.09
	assign (segid 3A4 and resid 245 and name N)	(segid 3A4 and resid 247 and name CB)	5.45	0.18	0.18
20	assign (segid 3A4 and resid 245 and name N)	(segid 3A4 and resid 247 and name N)	4.35	0.06	0.07
	assign (segid 3A4 and resid 245 and name N)	(segid 3A4 and resid 247 and name O)	6.86	0.06	0.05
	assign (segid 3A4 and resid 245 and name N)	(segid 3A4 and resid 248 and name C)	6.46	0.10	0.11
	assign (segid 3A4 and resid 245 and name N)	(segid 3A4 and resid 248 and name CA)	5.64	0.06	0.07
	assign (segid 3A4 and resid 245 and name N)	(segid 3A4 and resid 248 and name CB)	5.10	0.16	0.15
	assign (segid 3A4 and resid 245 and name N)	(segid 3A4 and resid 248 and name N)	4.85	0.02	0.02
25	assign (segid 3A4 and resid 245 and name N)	(segid 3A4 and resid 248 and name O)	7.66	0.12	0.11
	assign (segid 3A4 and resid 245 and name N)	(segid 3A4 and resid 249 and name CA)	7.22	0.12	0.13
	assign (segid 3A4 and resid 245 and name N)	(segid 3A4 and resid 249 and name N)	6.11	0.11	0.11
	assign (segid 3A4 and resid 245 and name N)	(segid 3A4 and resid 249 and name CB)	3.30	0.06	0.07
	assign (segid 3A4 and resid 245 and name O)	(segid 3A4 and resid 245 and name C)	3.04	0.08	0.07
30	assign (segid 3A4 and resid 245 and name O)	(segid 3A4 and resid 246 and name CA)	2.78	0.02	0.02
	assign (segid 3A4 and resid 245 and name O)	(segid 3A4 and resid 246 and name CB)	4.26	0.03	0.03
	assign (segid 3A4 and resid 245 and name O)	(segid 3A4 and resid 246 and name N)	2.25	0.01	0.01
	assign (segid 3A4 and resid 245 and name O)	(segid 3A4 and resid 246 and name O)	3.59	0.07	0.08
35	assign (segid 3A4 and resid 245 and name O)	(segid 3A4 and resid 247 and name C)	4.06	0.19	0.19
	assign (segid 3A4 and resid 245 and name O)	(segid 3A4 and resid 247 and name CA)	4.38	0.20	0.19
	assign (segid 3A4 and resid 245 and name O)	(segid 3A4 and resid 247 and name CB)	5.35	0.24	0.23
	assign (segid 3A4 and resid 245 and name O)	(segid 3A4 and resid 247 and name N)	3.43	0.18	0.18
	assign (segid 3A4 and resid 245 and name O)	(segid 3A4 and resid 247 and name O)	4.93	0.19	0.19
40	assign (segid 3A4 and resid 245 and name O)	(segid 3A4 and resid 248 and name C)	3.81	0.12	0.12
	assign (segid 3A4 and resid 245 and name O)	(segid 3A4 and resid 248 and name CA)	3.78	0.13	0.13
	assign (segid 3A4 and resid 245 and name O)	(segid 3A4 and resid 248 and name CB)	3.67	0.14	0.14
	assign (segid 3A4 and resid 245 and name O)	(segid 3A4 and resid 248 and name N)	3.32	0.17	0.17
	assign (segid 3A4 and resid 245 and name O)	(segid 3A4 and resid 248 and name O)	4.97	0.14	0.14
45	assign (segid 3A4 and resid 245 and name O)	(segid 3A4 and resid 249 and name C)	5.00	0.10	0.11
	assign (segid 3A4 and resid 245 and name O)	(segid 3A4 and resid 249 and name CA)	3.84	0.13	0.13
	assign (segid 3A4 and resid 245 and name O)	(segid 3A4 and resid 249 and name N)	2.99	0.10	0.10
	assign (segid 3A4 and resid 245 and name O)	(segid 3A4 and resid 249 and name O)	6.12	0.10	0.10
	assign (segid 3A4 and resid 245 and name O)	(segid 3A4 and resid 250 and name C)	7.25	0.13	0.13
50	assign (segid 3A4 and resid 245 and name O)	(segid 3A4 and resid 250 and name CA)	6.41	0.14	0.13
	assign (segid 3A4 and resid 245 and name O)	(segid 3A4 and resid 250 and name CB)	6.67	0.19	0.18
	assign (segid 3A4 and resid 245 and name O)	(segid 3A4 and resid 250 and name N)	5.05	0.12	0.11
	assign (segid 3A4 and resid 245 and name O)	(segid 3A4 and resid 251 and name N)	6.93	0.15	0.16
	assign (segid 3A4 and resid 246 and name C)	(segid 3A4 and resid 246 and name CB)	2.51	0.03	0.03
	assign (segid 3A4 and resid 246 and name C)	(segid 3A4 and resid 246 and name O)	1.23	0.01	0.01
55	assign (segid 3A4 and resid 246 and name C)	(segid 3A4 and resid 247 and name C)	3.04	0.04	0.03
	assign (segid 3A4 and resid 246 and name C)	(segid 3A4 and resid 247 and name CA)	2.43	0.01	0.01
	assign (segid 3A4 and resid 246 and name C)	(segid 3A4 and resid 247 and name CB)	3.72	0.03	0.02
	assign (segid 3A4 and resid 246 and name C)	(segid 3A4 and resid 247 and name N)	1.32	0.00	0.01
	assign (segid 3A4 and resid 246 and name C)	(segid 3A4 and resid 247 and name O)	3.81	0.02	0.03
60	assign (segid 3A4 and resid 246 and name C)	(segid 3A4 and resid 248 and name C)	4.61	0.10	0.09
	assign (segid 3A4 and resid 246 and name C)	(segid 3A4 and resid 248 and name CA)	4.56	0.09	0.10
	assign (segid 3A4 and resid 246 and name C)	(segid 3A4 and resid 248 and name CB)	5.32	0.13	0.13
	assign (segid 3A4 and resid 246 and name C)	(segid 3A4 and resid 248 and name N)	3.39	0.08	0.08
	assign (segid 3A4 and resid 246 and name C)	(segid 3A4 and resid 248 and name O)	5.68	0.14	0.14
65	assign (segid 3A4 and resid 246 and name C)	(segid 3A4 and resid 249 and name C)	4.84	0.13	0.13
	assign (segid 3A4 and resid 246 and name C)	(segid 3A4 and resid 249 and name CA)	4.53	0.09	0.09
	assign (segid 3A4 and resid 246 and name C)	(segid 3A4 and resid 249 and name N)	3.83	0.07	0.08
	assign (segid 3A4 and resid 246 and name C)	(segid 3A4 and resid 249 and name O)	6.05	0.14	0.14
	assign (segid 3A4 and resid 246 and name C)	(segid 3A4 and resid 250 and name C)	6.11	0.22	0.21
70	assign (segid 3A4 and resid 246 and name C)	(segid 3A4 and resid 250 and name CA)	5.02	0.23	0.23
	assign (segid 3A4 and resid 246 and name C)	(segid 3A4 and resid 250 and name CB)	4.62	0.27	0.27
	assign (segid 3A4 and resid 246 and name C)	(segid 3A4 and resid 250 and name N)	4.11	0.17	0.18
	assign (segid 3A4 and resid 246 and name C)	(segid 3A4 and resid 250 and name O)	7.25	0.22	0.23
	assign (segid 3A4 and resid 246 and name C)	(segid 3A4 and resid 251 and name CA)	7.32	0.16	0.16
75	assign (segid 3A4 and resid 246 and name C)	(segid 3A4 and resid 251 and name CB)	7.39	0.15	0.14
	assign (segid 3A4 and resid 246 and name C)	(segid 3A4 and resid 251 and name CG)	7.15	0.10	0.09
	assign (segid 3A4 and resid 246 and name C)	(segid 3A4 and resid 251 and name N)	6.02	0.16	0.17
	assign (segid 3A4 and resid 246 and name C)	(segid 3A4 and resid 246 and name C)	1.52	0.01	0.01
	assign (segid 3A4 and resid 246 and name CA)	(segid 3A4 and resid 246 and name CB)	1.53	0.01	0.01
80	assign (segid 3A4 and resid 246 and name CA)	(segid 3A4 and resid 246 and name O)	2.38	0.02	0.03
	assign (segid 3A4 and resid 246 and name CA)	(segid 3A4 and resid 247 and name C)	4.39	0.02	0.02
	assign (segid 3A4 and resid 246 and name CA)	(segid 3A4 and resid 247 and name CA)	3.81	0.01	0.01

	assign (segid 3A4 and resid 246 and name CA) (segid 3A4 and resid 247 and name CB)	4.89	0.04	0.04
	assign (segid 3A4 and resid 246 and name CA) (segid 3A4 and resid 247 and name N)	2.45	0.01	0.01
	assign (segid 3A4 and resid 246 and name CA) (segid 3A4 and resid 247 and name O)	5.25	0.03	0.02
	assign (segid 3A4 and resid 246 and name CA) (segid 3A4 and resid 248 and name C)	5.50	0.07	0.06
	assign (segid 3A4 and resid 246 and name CA) (segid 3A4 and resid 248 and name CA)	5.49	0.07	0.07
5	assign (segid 3A4 and resid 246 and name CA) (segid 3A4 and resid 248 and name CB)	5.92	0.12	0.12
	assign (segid 3A4 and resid 246 and name CA) (segid 3A4 and resid 248 and name N)	4.43	0.05	0.06
	assign (segid 3A4 and resid 246 and name CA) (segid 3A4 and resid 248 and name O)	6.62	0.10	0.10
	assign (segid 3A4 and resid 246 and name CA) (segid 3A4 and resid 249 and name C)	5.66	0.11	0.11
	assign (segid 3A4 and resid 246 and name CA) (segid 3A4 and resid 249 and name CA)	5.08	0.05	0.04
10	assign (segid 3A4 and resid 246 and name CA) (segid 3A4 and resid 249 and name N)	4.54	0.03	0.03
	assign (segid 3A4 and resid 246 and name CA) (segid 3A4 and resid 249 and name O)	6.84	0.12	0.13
	assign (segid 3A4 and resid 246 and name CA) (segid 3A4 and resid 250 and name C)	7.37	0.20	0.20
	assign (segid 3A4 and resid 246 and name CA) (segid 3A4 and resid 250 and name CA)	6.17	0.22	0.23
	assign (segid 3A4 and resid 246 and name CA) (segid 3A4 and resid 250 and name CB)	5.88	0.26	0.26
15	assign (segid 3A4 and resid 246 and name CA) (segid 3A4 and resid 250 and name N)	5.16	0.17	0.17
	assign (segid 3A4 and resid 246 and name CA) (segid 3A4 and resid 251 and name CA)	8.68	0.12	0.13
	assign (segid 3A4 and resid 246 and name CA) (segid 3A4 and resid 251 and name CB)	8.76	0.11	0.12
	assign (segid 3A4 and resid 246 and name CA) (segid 3A4 and resid 251 and name N)	7.36	0.14	0.13
	assign (segid 3A4 and resid 246 and name CA) (segid 3A4 and resid 252 and name CA)	10.00	0.12	0.12
20	assign (segid 3A4 and resid 246 and name CA) (segid 3A4 and resid 252 and name CB)	9.54	0.09	0.09
	assign (segid 3A4 and resid 246 and name CA) (segid 3A4 and resid 253 and name CA)	10.60	0.26	0.27
	assign (segid 3A4 and resid 246 and name CA) (segid 3A4 and resid 254 and name CA)	11.85	0.36	0.37
	assign (segid 3A4 and resid 246 and name CA) (segid 3A4 and resid 255 and name CA)	13.89	0.48	0.48
	assign (segid 3A4 and resid 246 and name CA) (segid 3A4 and resid 256 and name CA)	15.56	0.33	0.32
25	assign (segid 3A4 and resid 246 and name CA) (segid 3A4 and resid 257 and name CA)	17.20	0.45	0.44
	assign (segid 3A4 and resid 246 and name CA) (segid 3A4 and resid 258 and name CA)	18.50	0.39	0.38
	assign (segid 3A4 and resid 246 and name CA) (segid 3A4 and resid 258 and name CB)	17.75	0.44	0.45
	assign (segid 3A4 and resid 246 and name CA) (segid 3A4 and resid 389 and name CA)	16.58	0.54	0.54
	assign (segid 3A4 and resid 246 and name CA) (segid 3A4 and resid 389 and name CB)	16.32	0.72	0.72
30	assign (segid 3A4 and resid 246 and name CA) (segid 3A4 and resid 390 and name CA)	18.46	0.39	0.39
	assign (segid 3A4 and resid 246 and name CA) (segid 3A4 and resid 391 and name CA)	16.68	0.33	0.32
	assign (segid 3A4 and resid 246 and name CA) (segid 3A4 and resid 391 and name CB)	17.36	0.31	0.32
	assign (segid 3A4 and resid 246 and name CA) (segid 3A4 and resid 392 and name CA)	15.37	0.36	0.36
	assign (segid 3A4 and resid 246 and name CA) (segid 3A4 and resid 392 and name CB)	13.99	0.39	0.39
35	assign (segid 3A4 and resid 246 and name CA) (segid 3A4 and resid 393 and name CA)	16.15	0.41	0.41
	assign (segid 3A4 and resid 246 and name CA) (segid 3A4 and resid 396 and name CB)	18.55	0.56	0.57
	assign (segid 3A4 and resid 246 and name CB) (segid 3A4 and resid 247 and name C)	5.47	0.07	0.07
	assign (segid 3A4 and resid 246 and name CB) (segid 3A4 and resid 247 and name CA)	4.55	0.08	0.08
	assign (segid 3A4 and resid 246 and name CB) (segid 3A4 and resid 247 and name CB)	5.45	0.13	0.13
40	assign (segid 3A4 and resid 246 and name CB) (segid 3A4 and resid 247 and name N)	3.23	0.09	0.09
	assign (segid 3A4 and resid 246 and name CB) (segid 3A4 and resid 247 and name O)	6.28	0.05	0.06
	assign (segid 3A4 and resid 246 and name CB) (segid 3A4 and resid 248 and name C)	6.92	0.08	0.09
	assign (segid 3A4 and resid 246 and name CB) (segid 3A4 and resid 248 and name CA)	6.89	0.09	0.09
	assign (segid 3A4 and resid 246 and name CB) (segid 3A4 and resid 248 and name CB)	7.37	0.13	0.13
45	assign (segid 3A4 and resid 246 and name CB) (segid 3A4 and resid 248 and name N)	5.71	0.09	0.09
	assign (segid 3A4 and resid 246 and name CB) (segid 3A4 and resid 249 and name C)	6.82	0.15	0.15
	assign (segid 3A4 and resid 246 and name CB) (segid 3A4 and resid 249 and name CA)	6.41	0.06	0.06
	assign (segid 3A4 and resid 246 and name CB) (segid 3A4 and resid 249 and name N)	5.98	0.05	0.05
	assign (segid 3A4 and resid 246 and name CB) (segid 3A4 and resid 250 and name CA)	6.96	0.30	0.30
50	assign (segid 3A4 and resid 246 and name CB) (segid 3A4 and resid 250 and name CB)	6.40	0.34	0.35
	assign (segid 3A4 and resid 246 and name CB) (segid 3A4 and resid 250 and name N)	6.17	0.22	0.22
	assign (segid 3A4 and resid 246 and name CB) (segid 3A4 and resid 251 and name CA)	9.72	0.19	0.18
	assign (segid 3A4 and resid 246 and name CB) (segid 3A4 and resid 251 and name CB)	9.86	0.15	0.16
	assign (segid 3A4 and resid 246 and name CB) (segid 3A4 and resid 252 and name CA)	11.26	0.14	0.14
55	assign (segid 3A4 and resid 246 and name CB) (segid 3A4 and resid 252 and name CB)	10.88	0.07	0.08
	assign (segid 3A4 and resid 246 and name CB) (segid 3A4 and resid 253 and name CA)	11.56	0.31	0.31
	assign (segid 3A4 and resid 246 and name CB) (segid 3A4 and resid 254 and name CA)	12.57	0.48	0.48
	assign (segid 3A4 and resid 246 and name CB) (segid 3A4 and resid 255 and name CA)	14.85	0.50	0.49
	assign (segid 3A4 and resid 246 and name CB) (segid 3A4 and resid 256 and name CA)	16.64	0.32	0.31
60	assign (segid 3A4 and resid 246 and name CB) (segid 3A4 and resid 257 and name CA)	18.08	0.43	0.44
	assign (segid 3A4 and resid 246 and name CB) (segid 3A4 and resid 258 and name CB)	18.43	0.49	0.48
	assign (segid 3A4 and resid 246 and name CB) (segid 3A4 and resid 388 and name CA)	18.72	0.54	0.54
	assign (segid 3A4 and resid 246 and name CB) (segid 3A4 and resid 388 and name CB)	18.55	0.67	0.68
	assign (segid 3A4 and resid 246 and name CB) (segid 3A4 and resid 389 and name CA)	16.20	0.56	0.56
65	assign (segid 3A4 and resid 246 and name CB) (segid 3A4 and resid 389 and name CB)	15.87	0.74	0.73
	assign (segid 3A4 and resid 246 and name CB) (segid 3A4 and resid 390 and name CA)	18.35	0.43	0.44
	assign (segid 3A4 and resid 246 and name CB) (segid 3A4 and resid 391 and name CA)	16.87	0.38	0.37
	assign (segid 3A4 and resid 246 and name CB) (segid 3A4 and resid 391 and name CB)	17.64	0.37	0.37
	assign (segid 3A4 and resid 246 and name CB) (segid 3A4 and resid 392 and name CA)	15.68	0.41	0.41
70	assign (segid 3A4 and resid 246 and name CB) (segid 3A4 and resid 392 and name CB)	14.29	0.44	0.44
	assign (segid 3A4 and resid 246 and name CB) (segid 3A4 and resid 393 and name CA)	16.78	0.46	0.45
	assign (segid 3A4 and resid 246 and name C) (segid 3A4 and resid 246 and name C)	2.49	0.01	0.00
	assign (segid 3A4 and resid 246 and name N) (segid 3A4 and resid 246 and name CA)	1.46	0.00	0.00
	assign (segid 3A4 and resid 246 and name N) (segid 3A4 and resid 246 and name CB)	2.46	0.01	0.00
75	assign (segid 3A4 and resid 246 and name N) (segid 3A4 and resid 246 and name O)	3.54	0.03	0.02
	assign (segid 3A4 and resid 246 and name N) (segid 3A4 and resid 247 and name C)	4.70	0.03	0.03
	assign (segid 3A4 and resid 246 and name N) (segid 3A4 and resid 247 and name CA)	4.24	0.04	0.03
	assign (segid 3A4 and resid 246 and name N) (segid 3A4 and resid 247 and name CB)	5.02	0.10	0.09
	assign (segid 3A4 and resid 246 and name N) (segid 3A4 and resid 247 and name N)	2.84	0.04	0.04
80	assign (segid 3A4 and resid 246 and name N) (segid 3A4 and resid 247 and name O)	5.74	0.03	0.03
	assign (segid 3A4 and resid 246 and name N) (segid 3A4 and resid 248 and name C)	5.62	0.06	0.05
	assign (segid 3A4 and resid 246 and name N) (segid 3A4 and resid 248 and name CA)	5.36	0.06	0.05

	assign (segid 3A4 and resid 246 and name N)	(segid 3A4 and resid 248 and name CB)	5.42	0.12	0.12
	assign (segid 3A4 and resid 246 and name N)	(segid 3A4 and resid 248 and name N)	4.36	0.04	0.04
	assign (segid 3A4 and resid 246 and name N)	(segid 3A4 and resid 248 and name O)	6.82	0.07	0.06
	assign (segid 3A4 and resid 246 and name N)	(segid 3A4 and resid 249 and name C)	6.42	0.08	0.08
	assign (segid 3A4 and resid 246 and name N)	(segid 3A4 and resid 249 and name CA)	5.56	0.07	0.07
5	assign (segid 3A4 and resid 246 and name N)	(segid 3A4 and resid 249 and name N)	4.79	0.05	0.06
	assign (segid 3A4 and resid 246 and name N)	(segid 3A4 and resid 249 and name O)	7.61	0.09	0.08
	assign (segid 3A4 and resid 246 and name N)	(segid 3A4 and resid 250 and name CA)	7.22	0.17	0.18
	assign (segid 3A4 and resid 246 and name N)	(segid 3A4 and resid 250 and name CB)	7.03	0.24	0.25
	assign (segid 3A4 and resid 246 and name N)	(segid 3A4 and resid 250 and name N)	6.08	0.13	0.13
10	assign (segid 3A4 and resid 246 and name N)	(segid 3A4 and resid 246 and name CB)	3.23	0.05	0.06
	assign (segid 3A4 and resid 246 and name O)	(segid 3A4 and resid 247 and name C)	3.05	0.08	0.08
	assign (segid 3A4 and resid 246 and name O)	(segid 3A4 and resid 247 and name CA)	2.76	0.02	0.02
	assign (segid 3A4 and resid 246 and name O)	(segid 3A4 and resid 247 and name CB)	4.23	0.03	0.04
	assign (segid 3A4 and resid 246 and name O)	(segid 3A4 and resid 247 and name N)	2.24	0.01	0.01
15	assign (segid 3A4 and resid 246 and name O)	(segid 3A4 and resid 247 and name O)	3.44	0.06	0.05
	assign (segid 3A4 and resid 246 and name O)	(segid 3A4 and resid 248 and name C)	4.31	0.20	0.21
	assign (segid 3A4 and resid 246 and name O)	(segid 3A4 and resid 248 and name CA)	4.61	0.18	0.18
	assign (segid 3A4 and resid 246 and name O)	(segid 3A4 and resid 248 and name CB)	5.59	0.22	0.22
	assign (segid 3A4 and resid 246 and name O)	(segid 3A4 and resid 248 and name N)	3.64	0.15	0.16
20	assign (segid 3A4 and resid 246 and name O)	(segid 3A4 and resid 248 and name O)	5.22	0.26	0.27
	assign (segid 3A4 and resid 246 and name O)	(segid 3A4 and resid 249 and name C)	3.90	0.22	0.21
	assign (segid 3A4 and resid 246 and name O)	(segid 3A4 and resid 249 and name CA)	3.88	0.18	0.18
	assign (segid 3A4 and resid 246 and name O)	(segid 3A4 and resid 249 and name N)	3.48	0.18	0.18
	assign (segid 3A4 and resid 246 and name O)	(segid 3A4 and resid 249 and name O)	5.06	0.23	0.23
25	assign (segid 3A4 and resid 246 and name O)	(segid 3A4 and resid 250 and name C)	5.08	0.28	0.27
	assign (segid 3A4 and resid 246 and name O)	(segid 3A4 and resid 250 and name CA)	3.88	0.27	0.27
	assign (segid 3A4 and resid 246 and name O)	(segid 3A4 and resid 250 and name CB)	3.55	0.27	0.26
	assign (segid 3A4 and resid 246 and name O)	(segid 3A4 and resid 250 and name N)	3.05	0.25	0.25
	assign (segid 3A4 and resid 246 and name O)	(segid 3A4 and resid 250 and name O)	6.18	0.28	0.27
30	assign (segid 3A4 and resid 246 and name O)	(segid 3A4 and resid 251 and name CA)	6.55	0.23	0.22
	assign (segid 3A4 and resid 246 and name O)	(segid 3A4 and resid 251 and name CB)	6.83	0.21	0.21
	assign (segid 3A4 and resid 246 and name O)	(segid 3A4 and resid 251 and name CG)	6.71	0.14	0.15
	assign (segid 3A4 and resid 246 and name O)	(segid 3A4 and resid 251 and name N)	5.17	0.24	0.23
	assign (segid 3A4 and resid 246 and name O)	(segid 3A4 and resid 251 and name O)	7.12	0.24	0.24
35	assign (segid 3A4 and resid 246 and name O)	(segid 3A4 and resid 252 and name N)	2.49	0.03	0.03
	assign (segid 3A4 and resid 247 and name C)	(segid 3A4 and resid 247 and name CB)	2.49	0.03	0.03
	assign (segid 3A4 and resid 247 and name C)	(segid 3A4 and resid 247 and name O)	1.23	0.00	0.01
	assign (segid 3A4 and resid 247 and name C)	(segid 3A4 and resid 248 and name C)	2.97	0.03	0.04
	assign (segid 3A4 and resid 247 and name C)	(segid 3A4 and resid 248 and name CA)	2.44	0.02	0.01
	assign (segid 3A4 and resid 247 and name C)	(segid 3A4 and resid 248 and name CB)	3.71	0.02	0.03
40	assign (segid 3A4 and resid 247 and name C)	(segid 3A4 and resid 248 and name N)	1.33	0.01	0.01
	assign (segid 3A4 and resid 247 and name C)	(segid 3A4 and resid 248 and name O)	3.84	0.09	0.09
	assign (segid 3A4 and resid 247 and name C)	(segid 3A4 and resid 249 and name C)	4.42	0.06	0.07
	assign (segid 3A4 and resid 247 and name C)	(segid 3A4 and resid 249 and name CA)	4.36	0.11	0.10
	assign (segid 3A4 and resid 247 and name C)	(segid 3A4 and resid 249 and name N)	3.19	0.13	0.12
45	assign (segid 3A4 and resid 247 and name C)	(segid 3A4 and resid 249 and name O)	5.50	0.07	0.08
	assign (segid 3A4 and resid 247 and name C)	(segid 3A4 and resid 250 and name C)	4.78	0.08	0.08
	assign (segid 3A4 and resid 247 and name C)	(segid 3A4 and resid 250 and name CA)	4.44	0.09	0.10
	assign (segid 3A4 and resid 247 and name C)	(segid 3A4 and resid 250 and name CB)	4.28	0.21	0.20
	assign (segid 3A4 and resid 247 and name C)	(segid 3A4 and resid 250 and name N)	3.70	0.07	0.06
50	assign (segid 3A4 and resid 247 and name C)	(segid 3A4 and resid 250 and name O)	5.98	0.08	0.09
	assign (segid 3A4 and resid 247 and name C)	(segid 3A4 and resid 251 and name C)	6.13	0.15	0.14
	assign (segid 3A4 and resid 247 and name C)	(segid 3A4 and resid 251 and name CA)	5.04	0.14	0.14
	assign (segid 3A4 and resid 247 and name C)	(segid 3A4 and resid 251 and name CB)	4.68	0.16	0.16
	assign (segid 3A4 and resid 247 and name C)	(segid 3A4 and resid 251 and name CG)	4.34	0.15	0.14
55	assign (segid 3A4 and resid 247 and name C)	(segid 3A4 and resid 251 and name N)	4.08	0.09	0.10
	assign (segid 3A4 and resid 247 and name C)	(segid 3A4 and resid 251 and name O)	7.29	0.15	0.15
	assign (segid 3A4 and resid 247 and name C)	(segid 3A4 and resid 252 and name CA)	7.28	0.15	0.15
	assign (segid 3A4 and resid 247 and name C)	(segid 3A4 and resid 252 and name CB)	7.26	0.13	0.13
	assign (segid 3A4 and resid 247 and name C)	(segid 3A4 and resid 252 and name N)	6.01	0.16	0.16
60	assign (segid 3A4 and resid 247 and name C)	(segid 3A4 and resid 252 and name O)	7.50	0.24	0.23
	assign (segid 3A4 and resid 247 and name C)	(segid HEM and resid 1 and name CMD)	1.54	0.02	0.01
	assign (segid 3A4 and resid 247 and name CA)	(segid 3A4 and resid 247 and name C)	1.52	0.02	0.02
	assign (segid 3A4 and resid 247 and name CA)	(segid 3A4 and resid 247 and name CB)	2.40	0.02	0.01
	assign (segid 3A4 and resid 247 and name CA)	(segid 3A4 and resid 247 and name O)	4.39	0.03	0.04
65	assign (segid 3A4 and resid 247 and name CA)	(segid 3A4 and resid 248 and name C)	3.83	0.03	0.03
	assign (segid 3A4 and resid 247 and name CA)	(segid 3A4 and resid 248 and name CB)	4.88	0.05	0.06
	assign (segid 3A4 and resid 247 and name CA)	(segid 3A4 and resid 248 and name N)	2.45	0.03	0.03
	assign (segid 3A4 and resid 247 and name CA)	(segid 3A4 and resid 248 and name O)	5.32	0.10	0.11
	assign (segid 3A4 and resid 247 and name CA)	(segid 3A4 and resid 249 and name C)	5.39	0.07	0.08
70	assign (segid 3A4 and resid 247 and name CA)	(segid 3A4 and resid 249 and name CA)	5.37	0.10	0.10
	assign (segid 3A4 and resid 247 and name CA)	(segid 3A4 and resid 249 and name N)	4.32	0.11	0.11
	assign (segid 3A4 and resid 247 and name CA)	(segid 3A4 and resid 249 and name O)	6.52	0.09	0.10
	assign (segid 3A4 and resid 247 and name CA)	(segid 3A4 and resid 250 and name C)	5.63	0.15	0.14
	assign (segid 3A4 and resid 247 and name CA)	(segid 3A4 and resid 250 and name CA)	5.04	0.14	0.15
75	assign (segid 3A4 and resid 247 and name CA)	(segid 3A4 and resid 250 and name CB)	4.43	0.25	0.25
	assign (segid 3A4 and resid 247 and name CA)	(segid 3A4 and resid 250 and name N)	4.46	0.09	0.09
	assign (segid 3A4 and resid 247 and name CA)	(segid 3A4 and resid 251 and name C)	6.79	0.14	0.15
	assign (segid 3A4 and resid 247 and name CA)	(segid 3A4 and resid 251 and name CA)	6.17	0.14	0.15
80	assign (segid 3A4 and resid 247 and name CA)	(segid 3A4 and resid 251 and name CB)	5.89	0.16	0.16
	assign (segid 3A4 and resid 247 and name CA)	(segid 3A4 and resid 251 and name CG)	5.28	0.11	0.10
	assign (segid 3A4 and resid 247 and name CA)	(segid 3A4 and resid 251 and name N)	5.14	0.12	0.13

assign (segid 3A4 and resid 247 and name CA) (segid 3A4 and resid 252 and name CA) 8.66 0.15 0.14
 assign (segid 3A4 and resid 247 and name CA) (segid 3A4 and resid 252 and name CB) 8.68 0.11 0.11
 assign (segid 3A4 and resid 247 and name CA) (segid 3A4 and resid 252 and name N) 7.36 0.15 0.15
 assign (segid 3A4 and resid 247 and name CA) (segid 3A4 and resid 253 and name CA) 9.98 0.19 0.18
 5 assign (segid 3A4 and resid 247 and name CA) (segid 3A4 and resid 254 and name CA) 10.29 0.20 0.21
 assign (segid 3A4 and resid 247 and name CA) (segid 3A4 and resid 255 and name CA) 11.81 0.61 0.62
 assign (segid 3A4 and resid 247 and name CA) (segid 3A4 and resid 256 and name CA) 14.11 0.36 0.36
 assign (segid 3A4 and resid 247 and name CA) (segid 3A4 and resid 257 and name CA) 16.16 0.55 0.56
 assign (segid 3A4 and resid 247 and name CA) (segid 3A4 and resid 258 and name CA) 16.91 0.48 0.48
 10 assign (segid 3A4 and resid 247 and name CA) (segid 3A4 and resid 258 and name CB) 16.01 0.52 0.52
 assign (segid 3A4 and resid 247 and name CA) (segid 3A4 and resid 259 and name CA) 18.14 0.43 0.44
 assign (segid 3A4 and resid 247 and name CA) (segid 3A4 and resid 259 and name CB) 17.45 0.53 0.53
 assign (segid 3A4 and resid 247 and name CA) (segid 3A4 and resid 259 and name CB) 18.18 0.53 0.54
 assign (segid 3A4 and resid 247 and name CA) (segid 3A4 and resid 384 and name CA) 18.38 0.25 0.25
 15 assign (segid 3A4 and resid 247 and name CA) (segid 3A4 and resid 384 and name CB) 18.33 0.23 0.22
 assign (segid 3A4 and resid 247 and name CA) (segid 3A4 and resid 385 and name CA) 18.78 0.44 0.45
 assign (segid 3A4 and resid 247 and name CA) (segid 3A4 and resid 388 and name CA) 16.82 0.28 0.27
 assign (segid 3A4 and resid 247 and name CA) (segid 3A4 and resid 388 and name CB) 16.91 0.37 0.38
 assign (segid 3A4 and resid 247 and name CA) (segid 3A4 and resid 389 and name CA) 14.34 0.39 0.40
 20 assign (segid 3A4 and resid 247 and name CA) (segid 3A4 and resid 389 and name CB) 14.38 0.58 0.58
 assign (segid 3A4 and resid 247 and name CA) (segid 3A4 and resid 390 and name CA) 15.81 0.27 0.27
 assign (segid 3A4 and resid 247 and name CA) (segid 3A4 and resid 390 and name CB) 16.90 0.28 0.28
 assign (segid 3A4 and resid 247 and name CA) (segid 3A4 and resid 391 and name CA) 13.83 0.24 0.25
 assign (segid 3A4 and resid 247 and name CA) (segid 3A4 and resid 391 and name CB) 14.57 0.24 0.25
 25 assign (segid 3A4 and resid 247 and name CA) (segid 3A4 and resid 392 and name CA) 12.01 0.32 0.33
 assign (segid 3A4 and resid 247 and name CA) (segid 3A4 and resid 392 and name CB) 10.59 0.35 0.34
 assign (segid 3A4 and resid 247 and name CA) (segid 3A4 and resid 393 and name CA) 12.84 0.41 0.41
 assign (segid 3A4 and resid 247 and name CA) (segid 3A4 and resid 394 and name CA) 16.46 0.36 0.36
 assign (segid 3A4 and resid 247 and name CA) (segid 3A4 and resid 394 and name CB) 17.12 0.34 0.34
 30 assign (segid 3A4 and resid 247 and name CA) (segid 3A4 and resid 395 and name CA) 18.01 0.49 0.49
 assign (segid 3A4 and resid 247 and name CA) (segid 3A4 and resid 396 and name CA) 16.60 0.56 0.56
 assign (segid 3A4 and resid 247 and name CA) (segid 3A4 and resid 396 and name CB) 15.22 0.60 0.59
 assign (segid 3A4 and resid 247 and name CA) (segid 3A4 and resid 397 and name CA) 17.55 0.55 0.55
 assign (segid 3A4 and resid 247 and name CA) (segid 3A4 and resid 397 and name CB) 17.16 0.52 0.52
 35 assign (segid 3A4 and resid 247 and name CB) (segid 3A4 and resid 248 and name C) 5.37 0.06 0.06
 assign (segid 3A4 and resid 247 and name CB) (segid 3A4 and resid 248 and name CA) 4.44 0.05 0.05
 assign (segid 3A4 and resid 247 and name CB) (segid 3A4 and resid 248 and name CB) 5.32 0.08 0.08
 assign (segid 3A4 and resid 247 and name CB) (segid 3A4 and resid 248 and name N) 3.11 0.06 0.06
 assign (segid 3A4 and resid 247 and name CB) (segid 3A4 and resid 248 and name O) 6.25 0.10 0.11
 40 assign (segid 3A4 and resid 247 and name CB) (segid 3A4 and resid 249 and name C) 6.77 0.05 0.06
 assign (segid 3A4 and resid 247 and name CB) (segid 3A4 and resid 249 and name CA) 6.71 0.09 0.10
 assign (segid 3A4 and resid 247 and name CB) (segid 3A4 and resid 249 and name N) 5.53 0.10 0.11
 assign (segid 3A4 and resid 247 and name CB) (segid 3A4 and resid 249 and name O) 7.87 0.07 0.06
 assign (segid 3A4 and resid 247 and name CB) (segid 3A4 and resid 250 and name C) 6.72 0.07 0.08
 45 assign (segid 3A4 and resid 247 and name CB) (segid 3A4 and resid 250 and name CA) 6.34 0.11 0.10
 assign (segid 3A4 and resid 247 and name CB) (segid 3A4 and resid 250 and name CB) 5.64 0.23 0.23
 assign (segid 3A4 and resid 247 and name CB) (segid 3A4 and resid 250 and name N) 5.86 0.06 0.06
 assign (segid 3A4 and resid 247 and name CB) (segid 3A4 and resid 250 and name O) 7.85 0.09 0.09
 50 assign (segid 3A4 and resid 247 and name CB) (segid 3A4 and resid 251 and name CA) 6.87 0.13 0.12
 assign (segid 3A4 and resid 247 and name CB) (segid 3A4 and resid 251 and name CB) 6.31 0.17 0.16
 assign (segid 3A4 and resid 247 and name CB) (segid 3A4 and resid 251 and name CG) 5.41 0.16 0.16
 assign (segid 3A4 and resid 247 and name CB) (segid 3A4 and resid 251 and name N) 6.07 0.07 0.07
 assign (segid 3A4 and resid 247 and name CB) (segid 3A4 and resid 252 and name CA) 9.61 0.13 0.14
 55 assign (segid 3A4 and resid 247 and name CB) (segid 3A4 and resid 252 and name CB) 9.69 0.12 0.13
 assign (segid 3A4 and resid 247 and name CB) (segid 3A4 and resid 253 and name CA) 11.21 0.14 0.14
 assign (segid 3A4 and resid 247 and name CB) (segid 3A4 and resid 254 and name CA) 11.27 0.12 0.11
 assign (segid 3A4 and resid 247 and name CB) (segid 3A4 and resid 255 and name CA) 12.54 0.66 0.66
 assign (segid 3A4 and resid 247 and name CB) (segid 3A4 and resid 256 and name CA) 15.01 0.37 0.37
 60 assign (segid 3A4 and resid 247 and name CB) (segid 3A4 and resid 257 and name CA) 17.22 0.61 0.61
 assign (segid 3A4 and resid 247 and name CB) (segid 3A4 and resid 258 and name CA) 17.78 0.55 0.56
 assign (segid 3A4 and resid 247 and name CB) (segid 3A4 and resid 258 and name CB) 16.83 0.59 0.60
 assign (segid 3A4 and resid 247 and name CB) (segid 3A4 and resid 259 and name CA) 18.83 0.45 0.44
 assign (segid 3A4 and resid 247 and name CB) (segid 3A4 and resid 259 and name CB) 18.07 0.51 0.51
 65 assign (segid 3A4 and resid 247 and name CB) (segid 3A4 and resid 384 and name CA) 18.69 0.29 0.29
 assign (segid 3A4 and resid 247 and name CB) (segid 3A4 and resid 384 and name CB) 18.54 0.26 0.25
 assign (segid 3A4 and resid 247 and name CB) (segid 3A4 and resid 385 and name CA) 19.09 0.48 0.48
 assign (segid 3A4 and resid 247 and name CB) (segid 3A4 and resid 388 and name CA) 16.55 0.27 0.27
 assign (segid 3A4 and resid 247 and name CB) (segid 3A4 and resid 388 and name CB) 16.61 0.35 0.34
 70 assign (segid 3A4 and resid 247 and name CB) (segid 3A4 and resid 388 and name CB) 14.34 0.38 0.39
 assign (segid 3A4 and resid 247 and name CB) (segid 3A4 and resid 389 and name CB) 14.51 0.55 0.55
 assign (segid 3A4 and resid 247 and name CB) (segid 3A4 and resid 390 and name CA) 15.81 0.29 0.29
 assign (segid 3A4 and resid 247 and name CB) (segid 3A4 and resid 390 and name CB) 16.81 0.31 0.31
 assign (segid 3A4 and resid 247 and name CB) (segid 3A4 and resid 391 and name CA) 13.94 0.26 0.26
 75 assign (segid 3A4 and resid 247 and name CB) (segid 3A4 and resid 391 and name CB) 14.76 0.26 0.26
 assign (segid 3A4 and resid 247 and name CB) (segid 3A4 and resid 392 and name CA) 11.79 0.28 0.28
 assign (segid 3A4 and resid 247 and name CB) (segid 3A4 and resid 392 and name CB) 10.31 0.28 0.27
 assign (segid 3A4 and resid 247 and name CB) (segid 3A4 and resid 393 and name CA) 12.80 0.42 0.42
 80 assign (segid 3A4 and resid 247 and name CB) (segid 3A4 and resid 394 and name CA) 16.44 0.37 0.38
 assign (segid 3A4 and resid 247 and name CB) (segid 3A4 and resid 394 and name CB) 17.06 0.37 0.36
 assign (segid 3A4 and resid 247 and name CB) (segid 3A4 and resid 395 and name CA) 17.77 0.52 0.51
 assign (segid 3A4 and resid 247 and name CB) (segid 3A4 and resid 396 and name CA) 16.48 0.58 0.59
 assign (segid 3A4 and resid 247 and name CB) (segid 3A4 and resid 396 and name CB) 15.11 0.62 0.61
 assign (segid 3A4 and resid 247 and name CB) (segid 3A4 and resid 397 and name CA) 17.74 0.55 0.54

	assign (segid 3A4 and resid 247 and name CB)	(segid 3A4 and resid 397 and name CB)	17.41	0.51	0.51
	assign (segid 3A4 and resid 247 and name N)	(segid 3A4 and resid 217 and name C)	2.43	0.01	0.02
	assign (segid 3A4 and resid 247 and name N)	(segid 3A4 and resid 247 and name CA)	1.45	0.02	0.01
	assign (segid 3A4 and resid 247 and name N)	(segid 3A4 and resid 247 and name CB)	2.47	0.03	0.03
5	assign (segid 3A4 and resid 247 and name N)	(segid 3A4 and resid 247 and name O)	3.45	0.02	0.01
	assign (segid 3A4 and resid 247 and name N)	(segid 3A4 and resid 248 and name C)	4.67	0.05	0.05
	assign (segid 3A4 and resid 247 and name N)	(segid 3A4 and resid 248 and name CA)	4.21	0.05	0.05
	assign (segid 3A4 and resid 247 and name N)	(segid 3A4 and resid 248 and name CB)	4.97	0.09	0.10
	assign (segid 3A4 and resid 247 and name N)	(segid 3A4 and resid 248 and name N)	2.82	0.04	0.04
10	assign (segid 3A4 and resid 247 and name N)	(segid 3A4 and resid 248 and name O)	5.76	0.09	0.09
	assign (segid 3A4 and resid 247 and name N)	(segid 3A4 and resid 249 and name C)	5.52	0.08	0.09
	assign (segid 3A4 and resid 247 and name N)	(segid 3A4 and resid 249 and name CA)	5.23	0.10	0.09
	assign (segid 3A4 and resid 247 and name N)	(segid 3A4 and resid 249 and name N)	4.24	0.10	0.10
	assign (segid 3A4 and resid 247 and name N)	(segid 3A4 and resid 249 and name O)	6.74	0.10	0.10
	assign (segid 3A4 and resid 247 and name N)	(segid 3A4 and resid 250 and name C)	6.39	0.16	0.17
15	assign (segid 3A4 and resid 247 and name N)	(segid 3A4 and resid 250 and name CA)	5.54	0.18	0.18
	assign (segid 3A4 and resid 247 and name N)	(segid 3A4 and resid 250 and name CB)	5.01	0.26	0.27
	assign (segid 3A4 and resid 247 and name N)	(segid 3A4 and resid 250 and name N)	4.72	0.11	0.12
	assign (segid 3A4 and resid 247 and name N)	(segid 3A4 and resid 250 and name O)	7.58	0.17	0.17
	assign (segid 3A4 and resid 247 and name N)	(segid 3A4 and resid 251 and name CA)	7.23	0.13	0.13
20	assign (segid 3A4 and resid 247 and name N)	(segid 3A4 and resid 251 and name CB)	7.05	0.15	0.14
	assign (segid 3A4 and resid 247 and name N)	(segid 3A4 and resid 251 and name CG)	6.60	0.10	0.10
	assign (segid 3A4 and resid 247 and name N)	(segid 3A4 and resid 251 and name N)	6.07	0.12	0.12
	assign (segid 3A4 and resid 247 and name N)	(segid 3A4 and resid 247 and name CB)	3.30	0.07	0.08
	assign (segid 3A4 and resid 247 and name O)	(segid 3A4 and resid 248 and name C)	2.91	0.04	0.04
25	assign (segid 3A4 and resid 247 and name O)	(segid 3A4 and resid 248 and name CA)	2.77	0.03	0.03
	assign (segid 3A4 and resid 247 and name O)	(segid 3A4 and resid 248 and name CB)	4.26	0.03	0.04
	assign (segid 3A4 and resid 247 and name O)	(segid 3A4 and resid 248 and name N)	2.25	0.02	0.02
	assign (segid 3A4 and resid 247 and name O)	(segid 3A4 and resid 248 and name O)	3.42	0.13	0.13
	assign (segid 3A4 and resid 247 and name O)	(segid 3A4 and resid 249 and name C)	3.90	0.13	0.13
30	assign (segid 3A4 and resid 247 and name O)	(segid 3A4 and resid 249 and name CA)	4.22	0.16	0.15
	assign (segid 3A4 and resid 247 and name O)	(segid 3A4 and resid 249 and name N)	3.29	0.16	0.16
	assign (segid 3A4 and resid 247 and name O)	(segid 3A4 and resid 249 and name O)	4.83	0.13	0.14
	assign (segid 3A4 and resid 247 and name O)	(segid 3A4 and resid 250 and name C)	3.68	0.09	0.08
	assign (segid 3A4 and resid 247 and name O)	(segid 3A4 and resid 250 and name CA)	3.59	0.10	0.10
35	assign (segid 3A4 and resid 247 and name O)	(segid 3A4 and resid 250 and name CB)	3.53	0.20	0.19
	assign (segid 3A4 and resid 247 and name O)	(segid 3A4 and resid 250 and name N)	3.10	0.12	0.12
	assign (segid 3A4 and resid 247 and name O)	(segid 3A4 and resid 250 and name O)	4.85	0.09	0.09
	assign (segid 3A4 and resid 247 and name O)	(segid 3A4 and resid 251 and name C)	5.01	0.16	0.17
	assign (segid 3A4 and resid 247 and name O)	(segid 3A4 and resid 251 and name CA)	3.86	0.14	0.15
40	assign (segid 3A4 and resid 247 and name O)	(segid 3A4 and resid 251 and name CB)	3.64	0.15	0.15
	assign (segid 3A4 and resid 247 and name O)	(segid 3A4 and resid 251 and name CG)	3.40	0.11	0.12
	assign (segid 3A4 and resid 247 and name O)	(segid 3A4 and resid 251 and name N)	2.91	0.12	0.11
	assign (segid 3A4 and resid 247 and name O)	(segid 3A4 and resid 251 and name O)	6.15	0.17	0.16
	assign (segid 3A4 and resid 247 and name O)	(segid 3A4 and resid 252 and name C)	7.19	0.19	0.18
45	assign (segid 3A4 and resid 247 and name O)	(segid 3A4 and resid 252 and name CA)	6.38	0.17	0.17
	assign (segid 3A4 and resid 247 and name O)	(segid 3A4 and resid 252 and name CB)	6.56	0.15	0.14
	assign (segid 3A4 and resid 247 and name O)	(segid 3A4 and resid 252 and name N)	5.03	0.17	0.17
	assign (segid 3A4 and resid 247 and name O)	(segid 3A4 and resid 253 and name N)	6.90	0.18	0.17
	assign (segid 3A4 and resid 247 and name O)	(segid 3A4 and resid 254 and name N)	7.65	0.12	0.12
50	assign (segid 3A4 and resid 247 and name O)	(segid 3A4 and resid 1 and name CMD)	6.52	0.23	0.23
	assign (segid 3A4 and resid 248 and name C)	(segid 3A4 and resid 248 and name CB)	2.49	0.03	0.03
	assign (segid 3A4 and resid 248 and name C)	(segid 3A4 and resid 248 and name O)	1.24	0.01	0.01
	assign (segid 3A4 and resid 248 and name C)	(segid 3A4 and resid 249 and name C)	3.02	0.04	0.04
	assign (segid 3A4 and resid 248 and name C)	(segid 3A4 and resid 249 and name CA)	2.43	0.02	0.02
55	assign (segid 3A4 and resid 248 and name C)	(segid 3A4 and resid 249 and name N)	1.32	0.00	0.01
	assign (segid 3A4 and resid 248 and name C)	(segid 3A4 and resid 249 and name O)	3.85	0.04	0.03
	assign (segid 3A4 and resid 248 and name C)	(segid 3A4 and resid 250 and name C)	4.56	0.07	0.07
	assign (segid 3A4 and resid 248 and name C)	(segid 3A4 and resid 250 and name CA)	4.48	0.11	0.12
	assign (segid 3A4 and resid 248 and name C)	(segid 3A4 and resid 250 and name CB)	5.26	0.16	0.15
60	assign (segid 3A4 and resid 248 and name C)	(segid 3A4 and resid 250 and name N)	3.30	0.11	0.11
	assign (segid 3A4 and resid 248 and name C)	(segid 3A4 and resid 250 and name O)	5.63	0.06	0.07
	assign (segid 3A4 and resid 248 and name C)	(segid 3A4 and resid 251 and name C)	4.98	0.13	0.12
	assign (segid 3A4 and resid 248 and name C)	(segid 3A4 and resid 251 and name CA)	4.62	0.12	0.11
	assign (segid 3A4 and resid 248 and name C)	(segid 3A4 and resid 251 and name CB)	4.43	0.13	0.13
65	assign (segid 3A4 and resid 248 and name C)	(segid 3A4 and resid 251 and name CG)	5.02	0.18	0.18
	assign (segid 3A4 and resid 248 and name C)	(segid 3A4 and resid 251 and name N)	3.85	0.09	0.09
	assign (segid 3A4 and resid 248 and name C)	(segid 3A4 and resid 251 and name O)	6.19	0.13	0.12
	assign (segid 3A4 and resid 248 and name C)	(segid 3A4 and resid 252 and name C)	6.22	0.14	0.14
	assign (segid 3A4 and resid 248 and name C)	(segid 3A4 and resid 252 and name CA)	5.16	0.14	0.15
70	assign (segid 3A4 and resid 248 and name C)	(segid 3A4 and resid 252 and name CB)	4.70	0.15	0.15
	assign (segid 3A4 and resid 248 and name C)	(segid 3A4 and resid 252 and name N)	4.27	0.14	0.15
	assign (segid 3A4 and resid 248 and name C)	(segid 3A4 and resid 252 and name O)	7.39	0.15	0.15
	assign (segid 3A4 and resid 248 and name C)	(segid 3A4 and resid 253 and name CA)	7.35	0.15	0.15
	assign (segid 3A4 and resid 248 and name C)	(segid 3A4 and resid 253 and name N)	6.06	0.14	0.14
75	assign (segid 3A4 and resid 248 and name C)	(segid 3A4 and resid 254 and name N)	7.86	0.06	0.05
	assign (segid 3A4 and resid 248 and name CA)	(segid 3A4 and resid 248 and name C)	1.52	0.01	0.01
	assign (segid 3A4 and resid 248 and name CA)	(segid 3A4 and resid 248 and name CB)	1.53	0.01	0.00
	assign (segid 3A4 and resid 248 and name CA)	(segid 3A4 and resid 248 and name O)	2.39	0.02	0.02
80	assign (segid 3A4 and resid 248 and name CA)	(segid 3A4 and resid 249 and name C)	4.39	0.03	0.03
	assign (segid 3A4 and resid 248 and name CA)	(segid 3A4 and resid 249 and name CA)	3.81	0.03	0.02
	assign (segid 3A4 and resid 248 and name CA)	(segid 3A4 and resid 249 and name N)	2.44	0.03	0.02
	assign (segid 3A4 and resid 248 and name CA)	(segid 3A4 and resid 249 and name O)	5.29	0.03	0.04

	assign (segid 3A4 and resid 248 and name CA)	(segid 3A4 and resid 250 and name C)	5.47	0.07	0.08
	assign (segid 3A4 and resid 248 and name CA)	(segid 3A4 and resid 250 and name CA)	5.45	0.12	0.11
	assign (segid 3A4 and resid 248 and name CA)	(segid 3A4 and resid 250 and name CB)	5.89	0.19	0.20
	assign (segid 3A4 and resid 248 and name CA)	(segid 3A4 and resid 250 and name N)	4.38	0.10	0.09
	assign (segid 3A4 and resid 248 and name CA)	(segid 3A4 and resid 250 and name O)	6.60	0.06	0.06
5	assign (segid 3A4 and resid 248 and name CA)	(segid 3A4 and resid 251 and name C)	5.79	0.15	0.15
	assign (segid 3A4 and resid 248 and name CA)	(segid 3A4 and resid 251 and name CA)	5.17	0.15	0.15
	assign (segid 3A4 and resid 248 and name CA)	(segid 3A4 and resid 251 and name CB)	4.56	0.18	0.18
	assign (segid 3A4 and resid 248 and name CA)	(segid 3A4 and resid 251 and name CG)	4.78	0.25	0.26
	assign (segid 3A4 and resid 248 and name CA)	(segid 3A4 and resid 251 and name N)	4.56	0.10	0.09
10	assign (segid 3A4 and resid 248 and name CA)	(segid 3A4 and resid 251 and name O)	6.97	0.16	0.16
	assign (segid 3A4 and resid 248 and name CA)	(segid 3A4 and resid 252 and name C)	7.46	0.15	0.15
	assign (segid 3A4 and resid 248 and name CA)	(segid 3A4 and resid 252 and name CA)	6.29	0.16	0.17
	assign (segid 3A4 and resid 248 and name CA)	(segid 3A4 and resid 252 and name CB)	5.93	0.16	0.17
	assign (segid 3A4 and resid 248 and name CA)	(segid 3A4 and resid 252 and name N)	5.30	0.17	0.16
15	assign (segid 3A4 and resid 248 and name CA)	(segid 3A4 and resid 253 and name CA)	8.73	0.15	0.15
	assign (segid 3A4 and resid 248 and name CA)	(segid 3A4 and resid 253 and name N)	7.41	0.14	0.14
	assign (segid 3A4 and resid 248 and name CA)	(segid 3A4 and resid 254 and name CA)	9.97	0.06	0.06
	assign (segid 3A4 and resid 248 and name CA)	(segid 3A4 and resid 254 and name N)	10.60	0.73	0.73
	assign (segid 3A4 and resid 248 and name CA)	(segid 3A4 and resid 255 and name CA)	12.24	0.46	0.46
20	assign (segid 3A4 and resid 248 and name CA)	(segid 3A4 and resid 256 and name CA)	14.82	0.56	0.57
	assign (segid 3A4 and resid 248 and name CA)	(segid 3A4 and resid 257 and name CA)	16.15	0.48	0.49
	assign (segid 3A4 and resid 248 and name CA)	(segid 3A4 and resid 258 and name CA)	15.52	0.54	0.54
	assign (segid 3A4 and resid 248 and name CA)	(segid 3A4 and resid 258 and name CB)	16.89	0.44	0.44
	assign (segid 3A4 and resid 248 and name CA)	(segid 3A4 and resid 259 and name CA)	16.04	0.55	0.55
25	assign (segid 3A4 and resid 248 and name CA)	(segid 3A4 and resid 260 and name CA)	18.46	0.46	0.46
	assign (segid 3A4 and resid 248 and name CA)	(segid 3A4 and resid 260 and name CB)	17.94	0.52	0.51
	assign (segid 3A4 and resid 248 and name CA)	(segid 3A4 and resid 384 and name CA)	19.42	0.20	0.20
	assign (segid 3A4 and resid 248 and name CA)	(segid 3A4 and resid 388 and name CA)	19.65	0.20	0.21
30	assign (segid 3A4 and resid 248 and name CA)	(segid 3A4 and resid 389 and name CA)	17.01	0.36	0.36
	assign (segid 3A4 and resid 248 and name CA)	(segid 3A4 and resid 389 and name CB)	17.12	0.56	0.57
	assign (segid 3A4 and resid 248 and name CA)	(segid 3A4 and resid 390 and name CA)	17.82	0.21	0.22
	assign (segid 3A4 and resid 248 and name CA)	(segid 3A4 and resid 390 and name CB)	18.87	0.23	0.23
	assign (segid 3A4 and resid 248 and name CA)	(segid 3A4 and resid 391 and name CA)	15.19	0.25	0.25
35	assign (segid 3A4 and resid 248 and name CA)	(segid 3A4 and resid 391 and name CB)	15.62	0.29	0.28
	assign (segid 3A4 and resid 248 and name CA)	(segid 3A4 and resid 392 and name CA)	13.24	0.37	0.37
	assign (segid 3A4 and resid 248 and name CA)	(segid 3A4 and resid 392 and name CB)	11.97	0.39	0.40
	assign (segid 3A4 and resid 248 and name CA)	(segid 3A4 and resid 393 and name CA)	12.98	0.38	0.37
	assign (segid 3A4 and resid 248 and name CA)	(segid 3A4 and resid 394 and name CA)	16.74	0.36	0.37
40	assign (segid 3A4 and resid 248 and name CA)	(segid 3A4 and resid 394 and name CB)	17.68	0.36	0.36
	assign (segid 3A4 and resid 248 and name CA)	(segid 3A4 and resid 395 and name CA)	17.88	0.46	0.47
	assign (segid 3A4 and resid 248 and name CA)	(segid 3A4 and resid 396 and name CA)	15.74	0.51	0.52
	assign (segid 3A4 and resid 248 and name CA)	(segid 3A4 and resid 396 and name CB)	14.26	0.50	0.51
	assign (segid 3A4 and resid 248 and name CA)	(segid 3A4 and resid 397 and name CA)	16.74	0.60	0.59
45	assign (segid 3A4 and resid 248 and name CA)	(segid 3A4 and resid 397 and name CB)	16.59	0.57	0.58
	assign (segid 3A4 and resid 248 and name CA)	(segid 3A4 and resid 400 and name CB)	18.00	0.76	0.76
	assign (segid 3A4 and resid 248 and name CB)	(segid 3A4 and resid 249 and name C)	5.43	0.05	0.04
	assign (segid 3A4 and resid 248 and name CB)	(segid 3A4 and resid 249 and name CA)	4.49	0.07	0.06
	assign (segid 3A4 and resid 248 and name CB)	(segid 3A4 and resid 249 and name N)	3.18	0.07	0.06
50	assign (segid 3A4 and resid 248 and name CB)	(segid 3A4 and resid 249 and name O)	6.28	0.06	0.06
	assign (segid 3A4 and resid 248 and name CB)	(segid 3A4 and resid 250 and name C)	6.89	0.08	0.07
	assign (segid 3A4 and resid 248 and name CB)	(segid 3A4 and resid 250 and name CA)	6.82	0.10	0.09
	assign (segid 3A4 and resid 248 and name CB)	(segid 3A4 and resid 250 and name CB)	7.32	0.18	0.18
	assign (segid 3A4 and resid 248 and name CB)	(segid 3A4 and resid 250 and name N)	5.62	0.08	0.08
55	assign (segid 3A4 and resid 248 and name CB)	(segid 3A4 and resid 251 and name C)	6.95	0.16	0.17
	assign (segid 3A4 and resid 248 and name CB)	(segid 3A4 and resid 251 and name CA)	6.50	0.16	0.17
	assign (segid 3A4 and resid 248 and name CB)	(segid 3A4 and resid 251 and name CB)	5.80	0.21	0.22
	assign (segid 3A4 and resid 248 and name CB)	(segid 3A4 and resid 251 and name CG)	6.08	0.30	0.30
	assign (segid 3A4 and resid 248 and name CB)	(segid 3A4 and resid 251 and name N)	5.99	0.09	0.09
60	assign (segid 3A4 and resid 248 and name CB)	(segid 3A4 and resid 252 and name CA)	7.09	0.20	0.20
	assign (segid 3A4 and resid 248 and name CB)	(segid 3A4 and resid 252 and name CB)	6.48	0.22	0.22
	assign (segid 3A4 and resid 248 and name CB)	(segid 3A4 and resid 252 and name N)	6.31	0.18	0.18
	assign (segid 3A4 and resid 248 and name CB)	(segid 3A4 and resid 253 and name CA)	9.72	0.18	0.18
	assign (segid 3A4 and resid 248 and name CB)	(segid 3A4 and resid 254 and name CA)	11.27	0.10	0.10
65	assign (segid 3A4 and resid 248 and name CB)	(segid 3A4 and resid 255 and name CA)	11.71	0.77	0.77
	assign (segid 3A4 and resid 248 and name CB)	(segid 3A4 and resid 256 and name CA)	13.08	0.50	0.51
	assign (segid 3A4 and resid 248 and name CB)	(segid 3A4 and resid 257 and name CA)	15.78	0.56	0.55
	assign (segid 3A4 and resid 248 and name CB)	(segid 3A4 and resid 258 and name CA)	17.31	0.49	0.48
	assign (segid 3A4 and resid 248 and name CB)	(segid 3A4 and resid 258 and name CB)	16.75	0.55	0.55
70	assign (segid 3A4 and resid 248 and name CB)	(segid 3A4 and resid 259 and name CA)	17.91	0.44	0.44
	assign (segid 3A4 and resid 248 and name CB)	(segid 3A4 and resid 259 and name CB)	17.02	0.55	0.55
	assign (segid 3A4 and resid 248 and name CB)	(segid 3A4 and resid 260 and name CA)	19.30	0.48	0.47
	assign (segid 3A4 and resid 248 and name CB)	(segid 3A4 and resid 260 and name CB)	18.72	0.53	0.53
	assign (segid 3A4 and resid 248 and name CB)	(segid 3A4 and resid 389 and name CA)	18.47	0.35	0.35
75	assign (segid 3A4 and resid 248 and name CB)	(segid 3A4 and resid 389 and name CB)	18.59	0.55	0.56
	assign (segid 3A4 and resid 248 and name CB)	(segid 3A4 and resid 390 and name CA)	19.30	0.21	0.21
	assign (segid 3A4 and resid 248 and name CB)	(segid 3A4 and resid 391 and name CA)	16.65	0.26	0.27
	assign (segid 3A4 and resid 248 and name CB)	(segid 3A4 and resid 391 and name CB)	17.07	0.31	0.30
	assign (segid 3A4 and resid 248 and name CB)	(segid 3A4 and resid 392 and name CA)	14.59	0.36	0.37
80	assign (segid 3A4 and resid 248 and name CB)	(segid 3A4 and resid 392 and name CB)	13.32	0.38	0.39
	assign (segid 3A4 and resid 248 and name CB)	(segid 3A4 and resid 393 and name CA)	14.23	0.39	0.40
	assign (segid 3A4 and resid 248 and name CB)	(segid 3A4 and resid 394 and name CA)	18.02	0.38	0.38
	assign (segid 3A4 and resid 248 and name CB)	(segid 3A4 and resid 394 and name CB)	19.00	0.38	0.37

	assign (segid 3A4 and resid 248 and name CB)	(segid 3A4 and resid 395 and name CA)	18.98	0.48	0.48
	assign (segid 3A4 and resid 248 and name CB)	(segid 3A4 and resid 396 and name CA)	16.70	0.53	0.53
	assign (segid 3A4 and resid 248 and name CB)	(segid 3A4 and resid 396 and name CB)	15.20	0.51	0.52
	assign (segid 3A4 and resid 248 and name CB)	(segid 3A4 and resid 397 and name CA)	17.82	0.62	0.61
5	assign (segid 3A4 and resid 248 and name CB)	(segid 3A4 and resid 397 and name CB)	17.75	0.59	0.60
	assign (segid 3A4 and resid 248 and name N)	(segid 3A4 and resid 248 and name C)	2.45	0.01	0.01
	assign (segid 3A4 and resid 248 and name N)	(segid 3A4 and resid 248 and name CA)	1.46	0.00	0.01
	assign (segid 3A4 and resid 248 and name N)	(segid 3A4 and resid 248 and name CB)	2.46	0.03	0.03
	assign (segid 3A4 and resid 248 and name N)	(segid 3A4 and resid 248 and name O)	3.50	0.05	0.05
10	assign (segid 3A4 and resid 248 and name N)	(segid 3A4 and resid 249 and name C)	4.67	0.04	0.03
	assign (segid 3A4 and resid 248 and name N)	(segid 3A4 and resid 249 and name CA)	4.19	0.06	0.05
	assign (segid 3A4 and resid 248 and name N)	(segid 3A4 and resid 249 and name N)	2.79	0.07	0.07
	assign (segid 3A4 and resid 248 and name N)	(segid 3A4 and resid 249 and name O)	5.74	0.05	0.06
	assign (segid 3A4 and resid 248 and name N)	(segid 3A4 and resid 250 and name C)	5.59	0.07	0.06
15	assign (segid 3A4 and resid 248 and name N)	(segid 3A4 and resid 250 and name CA)	5.29	0.10	0.11
	assign (segid 3A4 and resid 248 and name N)	(segid 3A4 and resid 250 and name CB)	5.38	0.20	0.21
	assign (segid 3A4 and resid 248 and name N)	(segid 3A4 and resid 250 and name N)	4.28	0.08	0.08
	assign (segid 3A4 and resid 248 and name N)	(segid 3A4 and resid 250 and name O)	6.79	0.06	0.06
	assign (segid 3A4 and resid 248 and name N)	(segid 3A4 and resid 251 and name C)	6.52	0.15	0.14
20	assign (segid 3A4 and resid 248 and name N)	(segid 3A4 and resid 251 and name CA)	5.63	0.14	0.14
	assign (segid 3A4 and resid 248 and name N)	(segid 3A4 and resid 251 and name CB)	5.10	0.18	0.18
	assign (segid 3A4 and resid 248 and name N)	(segid 3A4 and resid 251 and name CG)	4.96	0.22	0.21
	assign (segid 3A4 and resid 248 and name N)	(segid 3A4 and resid 251 and name N)	4.80	0.08	0.08
	assign (segid 3A4 and resid 248 and name N)	(segid 3A4 and resid 252 and name CA)	7.32	0.15	0.15
25	assign (segid 3A4 and resid 248 and name N)	(segid 3A4 and resid 252 and name CB)	7.07	0.14	0.15
	assign (segid 3A4 and resid 248 and name N)	(segid 3A4 and resid 252 and name N)	6.19	0.16	0.16
	assign (segid 3A4 and resid 248 and name N)	(segid 3A4 and resid 252 and name CB)	3.27	0.09	0.08
	assign (segid 3A4 and resid 248 and name O)	(segid 3A4 and resid 249 and name C)	3.00	0.09	0.09
	assign (segid 3A4 and resid 248 and name O)	(segid 3A4 and resid 249 and name CA)	2.76	0.04	0.04
30	assign (segid 3A4 and resid 248 and name O)	(segid 3A4 and resid 249 and name N)	2.24	0.02	0.02
	assign (segid 3A4 and resid 248 and name O)	(segid 3A4 and resid 249 and name O)	3.45	0.07	0.07
	assign (segid 3A4 and resid 248 and name O)	(segid 3A4 and resid 250 and name C)	4.17	0.19	0.20
	assign (segid 3A4 and resid 248 and name O)	(segid 3A4 and resid 250 and name CA)	4.45	0.21	0.21
	assign (segid 3A4 and resid 248 and name O)	(segid 3A4 and resid 250 and name CB)	5.45	0.23	0.23
35	assign (segid 3A4 and resid 248 and name O)	(segid 3A4 and resid 250 and name N)	3.49	0.17	0.18
	assign (segid 3A4 and resid 248 and name O)	(segid 3A4 and resid 250 and name O)	5.09	0.17	0.18
	assign (segid 3A4 and resid 248 and name O)	(segid 3A4 and resid 251 and name C)	3.99	0.12	0.12
	assign (segid 3A4 and resid 248 and name O)	(segid 3A4 and resid 251 and name CA)	3.91	0.16	0.16
	assign (segid 3A4 and resid 248 and name O)	(segid 3A4 and resid 251 and name CB)	3.81	0.14	0.14
40	assign (segid 3A4 and resid 248 and name O)	(segid 3A4 and resid 251 and name CG)	4.73	0.23	0.24
	assign (segid 3A4 and resid 248 and name O)	(segid 3A4 and resid 251 and name N)	3.40	0.19	0.20
	assign (segid 3A4 and resid 248 and name O)	(segid 3A4 and resid 251 and name O)	5.16	0.13	0.12
	assign (segid 3A4 and resid 248 and name O)	(segid 3A4 and resid 252 and name C)	5.14	0.12	0.12
	assign (segid 3A4 and resid 248 and name O)	(segid 3A4 and resid 252 and name CA)	3.99	0.13	0.14
45	assign (segid 3A4 and resid 248 and name O)	(segid 3A4 and resid 252 and name CB)	3.60	0.18	0.17
	assign (segid 3A4 and resid 248 and name O)	(segid 3A4 and resid 252 and name N)	3.17	0.11	0.11
	assign (segid 3A4 and resid 248 and name O)	(segid 3A4 and resid 252 and name O)	6.28	0.13	0.13
	assign (segid 3A4 and resid 248 and name O)	(segid 3A4 and resid 253 and name C)	7.38	0.09	0.09
	assign (segid 3A4 and resid 248 and name O)	(segid 3A4 and resid 253 and name CA)	6.52	0.12	0.12
50	assign (segid 3A4 and resid 248 and name O)	(segid 3A4 and resid 253 and name N)	5.15	0.12	0.11
	assign (segid 3A4 and resid 248 and name O)	(segid 3A4 and resid 254 and name N)	7.07	0.10	0.09
	assign (segid 3A4 and resid 249 and name C)	(segid 3A4 and resid 249 and name O)	1.23	0.01	0.01
	assign (segid 3A4 and resid 249 and name C)	(segid 3A4 and resid 250 and name C)	3.03	0.04	0.04
	assign (segid 3A4 and resid 249 and name C)	(segid 3A4 and resid 250 and name CA)	2.42	0.01	0.01
55	assign (segid 3A4 and resid 249 and name C)	(segid 3A4 and resid 250 and name CB)	3.70	0.02	0.02
	assign (segid 3A4 and resid 249 and name C)	(segid 3A4 and resid 250 and name N)	1.32	0.01	0.01
	assign (segid 3A4 and resid 249 and name C)	(segid 3A4 and resid 251 and name C)	3.88	0.11	0.10
	assign (segid 3A4 and resid 249 and name C)	(segid 3A4 and resid 251 and name CA)	4.61	0.09	0.10
	assign (segid 3A4 and resid 249 and name C)	(segid 3A4 and resid 251 and name CB)	4.52	0.08	0.07
60	assign (segid 3A4 and resid 249 and name C)	(segid 3A4 and resid 251 and name CG)	5.28	0.08	0.07
	assign (segid 3A4 and resid 249 and name C)	(segid 3A4 and resid 251 and name N)	6.04	0.06	0.06
	assign (segid 3A4 and resid 249 and name C)	(segid 3A4 and resid 251 and name O)	3.31	0.06	0.07
	assign (segid 3A4 and resid 249 and name C)	(segid 3A4 and resid 252 and name C)	5.67	0.15	0.15
	assign (segid 3A4 and resid 249 and name C)	(segid 3A4 and resid 252 and name CA)	4.94	0.11	0.11
65	assign (segid 3A4 and resid 249 and name C)	(segid 3A4 and resid 252 and name CB)	4.62	0.10	0.10
	assign (segid 3A4 and resid 249 and name C)	(segid 3A4 and resid 252 and name N)	4.36	0.10	0.10
	assign (segid 3A4 and resid 249 and name C)	(segid 3A4 and resid 252 and name O)	3.91	0.11	0.11
	assign (segid 3A4 and resid 249 and name C)	(segid 3A4 and resid 253 and name C)	6.16	0.13	0.12
	assign (segid 3A4 and resid 249 and name C)	(segid 3A4 and resid 253 and name CA)	6.04	0.17	0.18
70	assign (segid 3A4 and resid 249 and name C)	(segid 3A4 and resid 253 and name N)	5.11	0.17	0.17
	assign (segid 3A4 and resid 249 and name C)	(segid 3A4 and resid 253 and name O)	4.18	0.14	0.14
	assign (segid 3A4 and resid 249 and name C)	(segid 3A4 and resid 254 and name N)	7.24	0.17	0.18
	assign (segid 3A4 and resid 249 and name C)	(segid 3A4 and resid 254 and name CA)	6.98	0.19	0.19
	assign (segid 3A4 and resid 249 and name C)	(segid 3A4 and resid 254 and name O)	5.77	0.17	0.18
75	assign (segid 3A4 and resid 249 and name CA)	(segid 3A4 and resid 249 and name C)	1.51	0.01	0.02
	assign (segid 3A4 and resid 249 and name CA)	(segid 3A4 and resid 249 and name O)	2.38	0.03	0.02
	assign (segid 3A4 and resid 249 and name CA)	(segid 3A4 and resid 250 and name C)	4.41	0.04	0.04
	assign (segid 3A4 and resid 249 and name CA)	(segid 3A4 and resid 250 and name CA)	3.80	0.01	0.01
	assign (segid 3A4 and resid 249 and name CA)	(segid 3A4 and resid 250 and name CB)	4.85	0.02	0.03
80	assign (segid 3A4 and resid 249 and name CA)	(segid 3A4 and resid 250 and name N)	2.43	0.01	0.01
	assign (segid 3A4 and resid 249 and name CA)	(segid 3A4 and resid 250 and name O)	5.33	0.10	0.10
	assign (segid 3A4 and resid 249 and name CA)	(segid 3A4 and resid 251 and name C)	5.58	0.11	0.10
	assign (segid 3A4 and resid 249 and name CA)	(segid 3A4 and resid 251 and name CA)	5.51	0.09	0.09

	assign (segid 3A4 and resid 249 and name CA)	(segid 3A4 and resid 251 and name CB)	5.94	0.10	0.11
	assign (segid 3A4 and resid 249 and name CA)	(segid 3A4 and resid 251 and name CG)	6.68	0.09	0.10
	assign (segid 3A4 and resid 249 and name CA)	(segid 3A4 and resid 251 and name N)	4.41	0.08	0.08
	assign (segid 3A4 and resid 249 and name CA)	(segid 3A4 and resid 251 and name O)	6.70	0.14	0.13
	assign (segid 3A4 and resid 249 and name CA)	(segid 3A4 and resid 252 and name C)	5.81	0.13	0.14
5	assign (segid 3A4 and resid 249 and name CA)	(segid 3A4 and resid 252 and name CA)	5.25	0.10	0.10
	assign (segid 3A4 and resid 249 and name CA)	(segid 3A4 and resid 252 and name CB)	4.58	0.10	0.10
	assign (segid 3A4 and resid 249 and name CA)	(segid 3A4 and resid 252 and name N)	4.68	0.11	0.12
	assign (segid 3A4 and resid 249 and name CA)	(segid 3A4 and resid 252 and name O)	7.04	0.15	0.14
10	assign (segid 3A4 and resid 249 and name CA)	(segid 3A4 and resid 253 and name C)	7.31	0.20	0.20
	assign (segid 3A4 and resid 249 and name CA)	(segid 3A4 and resid 253 and name CA)	6.22	0.21	0.20
	assign (segid 3A4 and resid 249 and name CA)	(segid 3A4 and resid 253 and name N)	5.21	0.18	0.18
	assign (segid 3A4 and resid 249 and name CA)	(segid 3A4 and resid 254 and name CA)	8.41	0.19	0.19
	assign (segid 3A4 and resid 249 and name CA)	(segid 3A4 and resid 254 and name N)	7.16	0.18	0.19
	assign (segid 3A4 and resid 249 and name CA)	(segid 3A4 and resid 255 and name CA)	9.89	0.49	0.50
15	assign (segid 3A4 and resid 249 and name CA)	(segid 3A4 and resid 256 and name CA)	10.90	0.40	0.39
	assign (segid 3A4 and resid 249 and name CA)	(segid 3A4 and resid 257 and name CA)	12.78	0.49	0.50
	assign (segid 3A4 and resid 249 and name CA)	(segid 3A4 and resid 258 and name CA)	14.60	0.39	0.40
	assign (segid 3A4 and resid 249 and name CA)	(segid 3A4 and resid 258 and name CB)	14.13	0.45	0.45
	assign (segid 3A4 and resid 249 and name CA)	(segid 3A4 and resid 259 and name CA)	15.99	0.36	0.36
20	assign (segid 3A4 and resid 249 and name CA)	(segid 3A4 and resid 259 and name CB)	15.41	0.52	0.51
	assign (segid 3A4 and resid 249 and name CA)	(segid 3A4 and resid 260 and name CA)	17.10	0.33	0.33
	assign (segid 3A4 and resid 249 and name CA)	(segid 3A4 and resid 260 and name CB)	16.39	0.36	0.35
	assign (segid 3A4 and resid 249 and name CA)	(segid 3A4 and resid 261 and name CA)	18.88	0.43	0.42
	assign (segid 3A4 and resid 249 and name CA)	(segid 3A4 and resid 319 and name CA)	18.07	0.63	0.62
25	assign (segid 3A4 and resid 249 and name CA)	(segid 3A4 and resid 319 and name CB)	17.15	0.53	0.52
	assign (segid 3A4 and resid 249 and name CA)	(segid 3A4 and resid 384 and name CA)	19.03	0.28	0.29
	assign (segid 3A4 and resid 249 and name CA)	(segid 3A4 and resid 384 and name CB)	19.17	0.32	0.33
	assign (segid 3A4 and resid 249 and name CA)	(segid 3A4 and resid 389 and name CA)	17.11	0.49	0.48
	assign (segid 3A4 and resid 249 and name CA)	(segid 3A4 and resid 389 and name CB)	16.92	0.70	0.69
30	assign (segid 3A4 and resid 249 and name CA)	(segid 3A4 and resid 390 and name CA)	18.04	0.33	0.32
	assign (segid 3A4 and resid 249 and name CA)	(segid 3A4 and resid 390 and name CB)	19.27	0.32	0.31
	assign (segid 3A4 and resid 249 and name CA)	(segid 3A4 and resid 391 and name CA)	15.42	0.34	0.33
	assign (segid 3A4 and resid 249 and name CA)	(segid 3A4 and resid 391 and name CB)	15.69	0.35	0.34
	assign (segid 3A4 and resid 249 and name CA)	(segid 3A4 and resid 392 and name CA)	14.34	0.44	0.45
35	assign (segid 3A4 and resid 249 and name CA)	(segid 3A4 and resid 392 and name CB)	13.23	0.51	0.50
	assign (segid 3A4 and resid 249 and name CA)	(segid 3A4 and resid 393 and name CA)	13.95	0.35	0.36
	assign (segid 3A4 and resid 249 and name CA)	(segid 3A4 and resid 394 and name CA)	17.44	0.34	0.34
	assign (segid 3A4 and resid 249 and name CA)	(segid 3A4 and resid 394 and name CB)	18.37	0.34	0.35
	assign (segid 3A4 and resid 249 and name CA)	(segid 3A4 and resid 395 and name CA)	19.19	0.39	0.39
40	assign (segid 3A4 and resid 249 and name CA)	(segid 3A4 and resid 396 and name CA)	17.02	0.40	0.40
	assign (segid 3A4 and resid 249 and name CA)	(segid 3A4 and resid 396 and name CB)	15.63	0.40	0.40
	assign (segid 3A4 and resid 249 and name CA)	(segid 3A4 and resid 397 and name CA)	17.18	0.49	0.49
	assign (segid 3A4 and resid 249 and name CA)	(segid 3A4 and resid 397 and name CB)	16.82	0.48	0.48
	assign (segid 3A4 and resid 249 and name CA)	(segid 3A4 and resid 400 and name CB)	18.51	0.61	0.61
45	assign (segid 3A4 and resid 249 and name CA)	(segid 3A4 and resid 249 and name C)	2.42	0.01	0.02
	assign (segid 3A4 and resid 249 and name N)	(segid 3A4 and resid 249 and name CA)	1.45	0.01	0.01
	assign (segid 3A4 and resid 249 and name N)	(segid 3A4 and resid 249 and name C)	3.46	0.03	0.03
	assign (segid 3A4 and resid 249 and name N)	(segid 3A4 and resid 250 and name C)	4.67	0.04	0.04
	assign (segid 3A4 and resid 249 and name N)	(segid 3A4 and resid 250 and name CA)	4.18	0.04	0.03
50	assign (segid 3A4 and resid 249 and name N)	(segid 3A4 and resid 250 and name CB)	4.95	0.09	0.08
	assign (segid 3A4 and resid 249 and name N)	(segid 3A4 and resid 250 and name N)	2.78	0.04	0.04
	assign (segid 3A4 and resid 249 and name N)	(segid 3A4 and resid 250 and name O)	5.76	0.07	0.07
	assign (segid 3A4 and resid 249 and name N)	(segid 3A4 and resid 251 and name C)	5.69	0.13	0.13
	assign (segid 3A4 and resid 249 and name N)	(segid 3A4 and resid 251 and name CA)	5.34	0.12	0.13
55	assign (segid 3A4 and resid 249 and name N)	(segid 3A4 and resid 251 and name CB)	5.43	0.15	0.15
	assign (segid 3A4 and resid 249 and name N)	(segid 3A4 and resid 251 and name CG)	5.96	0.14	0.14
	assign (segid 3A4 and resid 249 and name N)	(segid 3A4 and resid 251 and name N)	4.30	0.10	0.10
	assign (segid 3A4 and resid 249 and name N)	(segid 3A4 and resid 251 and name O)	6.89	0.14	0.13
	assign (segid 3A4 and resid 249 and name N)	(segid 3A4 and resid 252 and name C)	6.55	0.13	0.13
60	assign (segid 3A4 and resid 249 and name N)	(segid 3A4 and resid 252 and name CA)	5.72	0.12	0.12
	assign (segid 3A4 and resid 249 and name N)	(segid 3A4 and resid 252 and name CB)	5.14	0.10	0.10
	assign (segid 3A4 and resid 249 and name N)	(segid 3A4 and resid 252 and name N)	4.93	0.14	0.14
	assign (segid 3A4 and resid 249 and name N)	(segid 3A4 and resid 252 and name O)	7.77	0.14	0.14
	assign (segid 3A4 and resid 249 and name N)	(segid 3A4 and resid 253 and name CA)	7.28	0.18	0.19
65	assign (segid 3A4 and resid 249 and name N)	(segid 3A4 and resid 253 and name N)	6.14	0.16	0.16
	assign (segid 3A4 and resid 249 and name O)	(segid 3A4 and resid 250 and name C)	3.00	0.05	0.05
	assign (segid 3A4 and resid 249 and name O)	(segid 3A4 and resid 250 and name CA)	2.76	0.03	0.03
	assign (segid 3A4 and resid 249 and name O)	(segid 3A4 and resid 250 and name CB)	4.24	0.01	0.02
	assign (segid 3A4 and resid 249 and name O)	(segid 3A4 and resid 250 and name N)	2.24	0.01	0.02
70	assign (segid 3A4 and resid 249 and name O)	(segid 3A4 and resid 250 and name O)	3.50	0.13	0.13
	assign (segid 3A4 and resid 249 and name O)	(segid 3A4 and resid 251 and name C)	4.18	0.12	0.12
	assign (segid 3A4 and resid 249 and name O)	(segid 3A4 and resid 251 and name CA)	4.45	0.09	0.10
	assign (segid 3A4 and resid 249 and name O)	(segid 3A4 and resid 251 and name CB)	5.43	0.10	0.11
	assign (segid 3A4 and resid 249 and name O)	(segid 3A4 and resid 251 and name CG)	6.41	0.10	0.09
75	assign (segid 3A4 and resid 249 and name O)	(segid 3A4 and resid 251 and name N)	3.48	0.07	0.08
	assign (segid 3A4 and resid 249 and name O)	(segid 3A4 and resid 251 and name O)	5.09	0.21	0.21
	assign (segid 3A4 and resid 249 and name O)	(segid 3A4 and resid 252 and name C)	3.89	0.13	0.12
	assign (segid 3A4 and resid 249 and name O)	(segid 3A4 and resid 252 and name CA)	3.83	0.09	0.09
	assign (segid 3A4 and resid 249 and name O)	(segid 3A4 and resid 252 and name CB)	3.63	0.10	0.10
80	assign (segid 3A4 and resid 249 and name O)	(segid 3A4 and resid 252 and name N)	3.39	0.10	0.10
	assign (segid 3A4 and resid 249 and name O)	(segid 3A4 and resid 252 and name O)	5.08	0.14	0.14
	assign (segid 3A4 and resid 249 and name O)	(segid 3A4 and resid 253 and name C)	4.95	0.19	0.20

	assign (segid 3A4 and resid 249 and name O) (segid 3A4 and resid 253 and name CA)	3.97	0.18	0.18
	assign (segid 3A4 and resid 249 and name O) (segid 3A4 and resid 253 and name N)	3.02	0.16	0.16
	assign (segid 3A4 and resid 249 and name O) (segid 3A4 and resid 253 and name O)	6.12	0.19	0.19
	assign (segid 3A4 and resid 249 and name O) (segid 3A4 and resid 254 and name C)	7.06	0.22	0.23
5	assign (segid 3A4 and resid 249 and name O) (segid 3A4 and resid 254 and name CA)	6.16	0.22	0.22
	assign (segid 3A4 and resid 249 and name O) (segid 3A4 and resid 254 and name N)	4.85	0.20	0.21
	assign (segid 3A4 and resid 249 and name O) (segid 3A4 and resid 255 and name N)	6.75	0.36	0.36
	assign (segid 3A4 and resid 249 and name O) (segid 3A4 and resid 24 and name CB)	2.51	0.03	0.03
	assign (segid 3A4 and resid 24 and name C) (segid 3A4 and resid 24 and name O)	1.23	0.00	0.00
	assign (segid 3A4 and resid 24 and name C) (segid 3A4 and resid 25 and name C)	3.32	0.16	0.17
10	assign (segid 3A4 and resid 24 and name C) (segid 3A4 and resid 25 and name CA)	2.43	0.02	0.02
	assign (segid 3A4 and resid 24 and name C) (segid 3A4 and resid 25 and name N)	1.33	0.02	0.01
	assign (segid 3A4 and resid 24 and name C) (segid 3A4 and resid 25 and name O)	3.70	0.31	0.30
	assign (segid 3A4 and resid 24 and name C) (segid 3A4 and resid 26 and name C)	5.75	0.58	0.59
	assign (segid 3A4 and resid 24 and name C) (segid 3A4 and resid 26 and name CA)	5.39	0.48	0.47
15	assign (segid 3A4 and resid 24 and name C) (segid 3A4 and resid 26 and name N)	4.18	0.50	0.50
	assign (segid 3A4 and resid 24 and name C) (segid 3A4 and resid 26 and name O)	6.32	0.78	0.78
	assign (segid 3A4 and resid 24 and name C) (segid 3A4 and resid 29 and name C)	6.08	0.26	0.26
	assign (segid 3A4 and resid 24 and name C) (segid 3A4 and resid 29 and name CA)	5.30	0.42	0.43
	assign (segid 3A4 and resid 24 and name C) (segid 3A4 and resid 29 and name N)	5.41	0.53	0.53
20	assign (segid 3A4 and resid 24 and name C) (segid 3A4 and resid 29 and name O)	7.10	0.25	0.25
	assign (segid 3A4 and resid 24 and name C) (segid 3A4 and resid 30 and name CA)	6.98	0.37	0.37
	assign (segid 3A4 and resid 24 and name C) (segid 3A4 and resid 30 and name N)	5.92	0.27	0.26
	assign (segid 3A4 and resid 24 and name C) (segid 3A4 and resid 30 and name O)	6.86	0.22	0.22
	assign (segid 3A4 and resid 24 and name C) (segid 3A4 and resid 24 and name C)	1.51	0.01	0.01
25	assign (segid 3A4 and resid 24 and name CA) (segid 3A4 and resid 24 and name CB)	1.53	0.01	0.00
	assign (segid 3A4 and resid 24 and name CA) (segid 3A4 and resid 24 and name O)	2.39	0.03	0.02
	assign (segid 3A4 and resid 24 and name CA) (segid 3A4 and resid 25 and name C)	4.57	0.12	0.12
	assign (segid 3A4 and resid 24 and name CA) (segid 3A4 and resid 25 and name CA)	3.79	0.02	0.03
	assign (segid 3A4 and resid 24 and name CA) (segid 3A4 and resid 25 and name N)	2.42	0.02	0.03
30	assign (segid 3A4 and resid 24 and name CA) (segid 3A4 and resid 25 and name O)	4.69	0.35	0.35
	assign (segid 3A4 and resid 24 and name CA) (segid 3A4 and resid 26 and name C)	6.72	0.68	0.68
	assign (segid 3A4 and resid 24 and name CA) (segid 3A4 and resid 26 and name CA)	6.57	0.51	0.51
	assign (segid 3A4 and resid 24 and name CA) (segid 3A4 and resid 26 and name N)	5.48	0.51	0.52
	assign (segid 3A4 and resid 24 and name CA) (segid 3A4 and resid 26 and name O)	7.21	0.92	0.92
35	assign (segid 3A4 and resid 24 and name CA) (segid 3A4 and resid 29 and name C)	5.35	0.08	0.09
	assign (segid 3A4 and resid 24 and name CA) (segid 3A4 and resid 29 and name CA)	4.49	0.22	0.22
	assign (segid 3A4 and resid 24 and name CA) (segid 3A4 and resid 29 and name N)	4.89	0.22	0.22
	assign (segid 3A4 and resid 24 and name CA) (segid 3A4 and resid 29 and name O)	6.48	0.08	0.08
	assign (segid 3A4 and resid 24 and name CA) (segid 3A4 and resid 30 and name C)	6.67	0.19	0.20
40	assign (segid 3A4 and resid 24 and name CA) (segid 3A4 and resid 30 and name CA)	6.34	0.25	0.25
	assign (segid 3A4 and resid 24 and name CA) (segid 3A4 and resid 30 and name N)	5.16	0.15	0.16
	assign (segid 3A4 and resid 24 and name CA) (segid 3A4 and resid 30 and name O)	6.02	0.09	0.09
	assign (segid 3A4 and resid 24 and name CA) (segid 3A4 and resid 31 and name CA)	8.66	0.21	0.21
	assign (segid 3A4 and resid 24 and name CA) (segid 3A4 and resid 31 and name CB)	9.90	0.29	0.29
45	assign (segid 3A4 and resid 24 and name CA) (segid 3A4 and resid 322 and name CA)	14.60	0.58	0.59
	assign (segid 3A4 and resid 24 and name CA) (segid 3A4 and resid 323 and name CA)	15.68	0.55	0.56
	assign (segid 3A4 and resid 24 and name CA) (segid 3A4 and resid 323 and name CB)	16.33	0.64	0.64
	assign (segid 3A4 and resid 24 and name CA) (segid 3A4 and resid 324 and name CA)	15.27	0.51	0.51
	assign (segid 3A4 and resid 24 and name CA) (segid 3A4 and resid 324 and name CB)	15.57	0.60	0.60
50	assign (segid 3A4 and resid 24 and name CA) (segid 3A4 and resid 325 and name CA)	16.75	0.37	0.37
	assign (segid 3A4 and resid 24 and name CA) (segid 3A4 and resid 325 and name CB)	16.17	0.36	0.36
	assign (segid 3A4 and resid 24 and name CA) (segid 3A4 and resid 32 and name CA)	10.25	0.46	0.46
	assign (segid 3A4 and resid 24 and name CA) (segid 3A4 and resid 32 and name CB)	9.71	0.55	0.55
	assign (segid 3A4 and resid 24 and name CA) (segid 3A4 and resid 331 and name CA)	18.88	0.32	0.31
55	assign (segid 3A4 and resid 24 and name CA) (segid 3A4 and resid 331 and name CB)	17.75	0.42	0.41
	assign (segid 3A4 and resid 24 and name CA) (segid 3A4 and resid 335 and name CA)	16.65	0.31	0.31
	assign (segid 3A4 and resid 24 and name CA) (segid 3A4 and resid 336 and name CA)	16.80	0.36	0.36
	assign (segid 3A4 and resid 24 and name CA) (segid 3A4 and resid 336 and name CB)	17.46	0.46	0.45
	assign (segid 3A4 and resid 24 and name CA) (segid 3A4 and resid 337 and name CA)	14.77	0.31	0.32
60	assign (segid 3A4 and resid 24 and name CA) (segid 3A4 and resid 337 and name CB)	14.78	0.46	0.47
	assign (segid 3A4 and resid 24 and name CA) (segid 3A4 and resid 338 and name CA)	15.40	0.40	0.40
	assign (segid 3A4 and resid 24 and name CA) (segid 3A4 and resid 338 and name CB)	14.84	0.54	0.54
	assign (segid 3A4 and resid 24 and name CA) (segid 3A4 and resid 339 and name CA)	17.06	0.43	0.43
	assign (segid 3A4 and resid 24 and name CA) (segid 3A4 and resid 339 and name CB)	18.36	0.42	0.42
65	assign (segid 3A4 and resid 24 and name CA) (segid 3A4 and resid 33 and name CA)	13.96	0.40	0.40
	assign (segid 3A4 and resid 24 and name CA) (segid 3A4 and resid 33 and name CB)	14.88	0.40	0.40
	assign (segid 3A4 and resid 24 and name CA) (segid 3A4 and resid 340 and name CA)	15.06	0.47	0.46
	assign (segid 3A4 and resid 24 and name CA) (segid 3A4 and resid 341 and name CA)	11.87	0.43	0.43
	assign (segid 3A4 and resid 24 and name CA) (segid 3A4 and resid 341 and name CB)	11.76	0.42	0.42
70	assign (segid 3A4 and resid 24 and name CA) (segid 3A4 and resid 342 and name CA)	10.82	0.51	0.51
	assign (segid 3A4 and resid 24 and name CA) (segid 3A4 and resid 343 and name CA)	11.57	0.32	0.32
	assign (segid 3A4 and resid 24 and name CA) (segid 3A4 and resid 343 and name CB)	12.86	0.26	0.26
	assign (segid 3A4 and resid 24 and name CA) (segid 3A4 and resid 344 and name CA)	11.83	0.51	0.50
	assign (segid 3A4 and resid 24 and name CA) (segid 3A4 and resid 344 and name CB)	10.74	0.55	0.56
75	assign (segid 3A4 and resid 24 and name CA) (segid 3A4 and resid 345 and name CA)	15.07	0.57	0.58
	assign (segid 3A4 and resid 24 and name CA) (segid 3A4 and resid 345 and name CB)	16.33	0.50	0.50
	assign (segid 3A4 and resid 24 and name CA) (segid 3A4 and resid 346 and name CA)	15.69	0.69	0.68
	assign (segid 3A4 and resid 24 and name CA) (segid 3A4 and resid 346 and name CB)	15.01	0.69	0.69
	assign (segid 3A4 and resid 24 and name CA) (segid 3A4 and resid 349 and name CB)	17.56	0.87	0.87
80	assign (segid 3A4 and resid 24 and name CA) (segid 3A4 and resid 34 and name CA)	15.84	0.58	0.57
	assign (segid 3A4 and resid 24 and name CA) (segid 3A4 and resid 34 and name CB)	15.37	0.62	0.63
	assign (segid 3A4 and resid 24 and name CA) (segid 3A4 and resid 38 and name CB)	18.51	0.25	0.25

	assign (segid 3A4 and resid 250 and name C) (segid 3A4 and resid 250 and name CB)	2.50	0.02	0.03
	assign (segid 3A4 and resid 250 and name C) (segid 3A4 and resid 250 and name O)	1.23	0.01	0.00
	assign (segid 3A4 and resid 250 and name C) (segid 3A4 and resid 251 and name C)	3.00	0.04	0.04
	assign (segid 3A4 and resid 250 and name C) (segid 3A4 and resid 251 and name CA)	2.42	0.01	0.01
	assign (segid 3A4 and resid 250 and name C) (segid 3A4 and resid 251 and name CB)	3.70	0.01	0.02
5	assign (segid 3A4 and resid 250 and name C) (segid 3A4 and resid 251 and name CG)	4.29	0.07	0.07
	assign (segid 3A4 and resid 250 and name C) (segid 3A4 and resid 251 and name N)	1.33	0.01	0.00
	assign (segid 3A4 and resid 250 and name C) (segid 3A4 and resid 251 and name O)	3.83	0.11	0.12
	assign (segid 3A4 and resid 250 and name C) (segid 3A4 and resid 252 and name C)	4.52	0.06	0.07
	assign (segid 3A4 and resid 250 and name C) (segid 3A4 and resid 252 and name CA)	4.44	0.09	0.10
10	assign (segid 3A4 and resid 250 and name C) (segid 3A4 and resid 252 and name CB)	5.15	0.11	0.11
	assign (segid 3A4 and resid 250 and name C) (segid 3A4 and resid 252 and name N)	3.27	0.12	0.12
	assign (segid 3A4 and resid 250 and name C) (segid 3A4 and resid 252 and name O)	5.50	0.10	0.09
	assign (segid 3A4 and resid 250 and name C) (segid 3A4 and resid 253 and name C)	4.90	0.07	0.07
	assign (segid 3A4 and resid 250 and name C) (segid 3A4 and resid 253 and name CA)	4.75	0.11	0.11
15	assign (segid 3A4 and resid 250 and name C) (segid 3A4 and resid 253 and name N)	3.95	0.06	0.07
	assign (segid 3A4 and resid 250 and name C) (segid 3A4 and resid 253 and name O)	6.09	0.06	0.07
	assign (segid 3A4 and resid 250 and name C) (segid 3A4 and resid 254 and name C)	5.71	0.23	0.22
	assign (segid 3A4 and resid 250 and name C) (segid 3A4 and resid 254 and name CA)	4.80	0.08	0.08
20	assign (segid 3A4 and resid 250 and name C) (segid 3A4 and resid 254 and name N)	4.03	0.06	0.06
	assign (segid 3A4 and resid 250 and name C) (segid 3A4 and resid 254 and name O)	6.85	0.22	0.22
	assign (segid 3A4 and resid 250 and name C) (segid 3A4 and resid 255 and name C)	6.67	0.46	0.47
	assign (segid 3A4 and resid 250 and name C) (segid 3A4 and resid 255 and name N)	5.49	0.38	0.37
	assign (segid 3A4 and resid 250 and name C) (segid HEM and resid 1 and name C1D)	6.38	0.31	0.31
	assign (segid 3A4 and resid 250 and name C) (segid HEM and resid 1 and name C2D)	6.10	0.37	0.38
25	assign (segid 3A4 and resid 250 and name C) (segid HEM and resid 1 and name C3C)	6.91	0.14	0.14
	assign (segid 3A4 and resid 250 and name C) (segid HEM and resid 1 and name C3D)	7.04	0.38	0.38
	assign (segid 3A4 and resid 250 and name C) (segid HEM and resid 1 and name C4C)	6.76	0.17	0.17
	assign (segid 3A4 and resid 250 and name C) (segid HEM and resid 1 and name CAC)	6.32	0.20	0.20
	assign (segid 3A4 and resid 250 and name C) (segid HEM and resid 1 and name CBC)	6.76	0.38	0.39
30	assign (segid 3A4 and resid 250 and name C) (segid HEM and resid 1 and name CHD)	6.00	0.26	0.25
	assign (segid 3A4 and resid 250 and name C) (segid HEM and resid 1 and name CMD)	5.32	0.44	0.43
	assign (segid 3A4 and resid 250 and name C) (segid HEM and resid 1 and name ND)	7.40	0.32	0.32
	assign (segid 3A4 and resid 250 and name CA) (segid 3A4 and resid 250 and name C)	1.53	0.01	0.00
35	assign (segid 3A4 and resid 250 and name CA) (segid 3A4 and resid 250 and name CB)	1.53	0.02	0.01
	assign (segid 3A4 and resid 250 and name CA) (segid 3A4 and resid 250 and name O)	2.38	0.01	0.02
	assign (segid 3A4 and resid 250 and name CA) (segid 3A4 and resid 251 and name C)	4.41	0.05	0.05
	assign (segid 3A4 and resid 250 and name CA) (segid 3A4 and resid 251 and name CA)	3.82	0.02	0.02
	assign (segid 3A4 and resid 250 and name CA) (segid 3A4 and resid 251 and name CB)	4.88	0.02	0.02
	assign (segid 3A4 and resid 250 and name CA) (segid 3A4 and resid 251 and name CG)	5.26	0.06	0.07
40	assign (segid 3A4 and resid 250 and name CA) (segid 3A4 and resid 251 and name N)	2.45	0.03	0.03
	assign (segid 3A4 and resid 250 and name CA) (segid 3A4 and resid 251 and name O)	5.30	0.13	0.12
	assign (segid 3A4 and resid 250 and name CA) (segid 3A4 and resid 252 and name C)	5.47	0.09	0.09
	assign (segid 3A4 and resid 250 and name CA) (segid 3A4 and resid 252 and name CA)	5.44	0.11	0.11
	assign (segid 3A4 and resid 250 and name CA) (segid 3A4 and resid 252 and name CB)	5.82	0.14	0.13
45	assign (segid 3A4 and resid 250 and name CA) (segid 3A4 and resid 252 and name N)	4.39	0.14	0.14
	assign (segid 3A4 and resid 250 and name CA) (segid 3A4 and resid 252 and name O)	6.53	0.12	0.11
	assign (segid 3A4 and resid 250 and name CA) (segid 3A4 and resid 253 and name C)	5.60	0.11	0.12
	assign (segid 3A4 and resid 250 and name CA) (segid 3A4 and resid 253 and name CA)	5.25	0.14	0.15
	assign (segid 3A4 and resid 250 and name CA) (segid 3A4 and resid 253 and name N)	4.63	0.08	0.08
50	assign (segid 3A4 and resid 250 and name CA) (segid 3A4 and resid 253 and name O)	6.80	0.11	0.11
	assign (segid 3A4 and resid 250 and name CA) (segid 3A4 and resid 254 and name C)	6.83	0.23	0.23
	assign (segid 3A4 and resid 250 and name CA) (segid 3A4 and resid 254 and name CA)	5.71	0.17	0.18
	assign (segid 3A4 and resid 250 and name CA) (segid 3A4 and resid 254 and name N)	4.88	0.15	0.14
	assign (segid 3A4 and resid 250 and name CA) (segid 3A4 and resid 255 and name CA)	8.03	0.42	0.42
55	assign (segid 3A4 and resid 250 and name CA) (segid 3A4 and resid 255 and name N)	6.77	0.35	0.36
	assign (segid 3A4 and resid 250 and name CA) (segid 3A4 and resid 256 and name CA)	9.97	0.23	0.23
	assign (segid 3A4 and resid 250 and name CA) (segid 3A4 and resid 257 and name CA)	11.44	0.67	0.67
	assign (segid 3A4 and resid 250 and name CA) (segid 3A4 and resid 258 and name CA)	12.39	0.54	0.54
60	assign (segid 3A4 and resid 250 and name CA) (segid 3A4 and resid 258 and name CB)	11.62	0.55	0.54
	assign (segid 3A4 and resid 250 and name CA) (segid 3A4 and resid 259 and name CA)	14.13	0.29	0.29
	assign (segid 3A4 and resid 250 and name CA) (segid 3A4 and resid 259 and name CB)	13.69	0.33	0.32
	assign (segid 3A4 and resid 250 and name CA) (segid 3A4 and resid 260 and name CA)	15.87	0.39	0.38
	assign (segid 3A4 and resid 250 and name CA) (segid 3A4 and resid 260 and name CB)	15.40	0.46	0.46
65	assign (segid 3A4 and resid 250 and name CA) (segid 3A4 and resid 261 and name CA)	17.19	0.51	0.52
	assign (segid 3A4 and resid 250 and name CA) (segid 3A4 and resid 262 and name CA)	18.39	0.35	0.35
	assign (segid 3A4 and resid 250 and name CA) (segid 3A4 and resid 262 and name CB)	17.69	0.29	0.29
	assign (segid 3A4 and resid 250 and name CA) (segid 3A4 and resid 318 and name CA)	17.01	0.56	0.56
	assign (segid 3A4 and resid 250 and name CA) (segid 3A4 and resid 318 and name CB)	16.40	0.69	0.68
70	assign (segid 3A4 and resid 250 and name CA) (segid 3A4 and resid 319 and name CA)	15.03	0.59	0.58
	assign (segid 3A4 and resid 250 and name CA) (segid 3A4 and resid 319 and name CB)	13.96	0.48	0.49
	assign (segid 3A4 and resid 250 and name CA) (segid 3A4 and resid 322 and name CA)	16.62	0.88	0.88
	assign (segid 3A4 and resid 250 and name CA) (segid 3A4 and resid 383 and name CA)	18.14	0.43	0.42
	assign (segid 3A4 and resid 250 and name CA) (segid 3A4 and resid 384 and name CA)	15.51	0.33	0.33
75	assign (segid 3A4 and resid 250 and name CA) (segid 3A4 and resid 384 and name CB)	15.71	0.34	0.33
	assign (segid 3A4 and resid 250 and name CA) (segid 3A4 and resid 385 and name CA)	16.22	0.44	0.44
	assign (segid 3A4 and resid 250 and name CA) (segid 3A4 and resid 386 and name CA)	18.42	0.35	0.35
	assign (segid 3A4 and resid 250 and name CA) (segid 3A4 and resid 387 and name CA)	18.68	0.46	0.46
	assign (segid 3A4 and resid 250 and name CA) (segid 3A4 and resid 388 and name CA)	16.71	0.32	0.33
80	assign (segid 3A4 and resid 250 and name CA) (segid 3A4 and resid 388 and name CB)	17.11	0.43	0.43
	assign (segid 3A4 and resid 250 and name CA) (segid 3A4 and resid 389 and name CA)	13.47	0.46	0.47
	assign (segid 3A4 and resid 250 and name CA) (segid 3A4 and resid 389 and name CB)	13.27	0.66	0.66
	assign (segid 3A4 and resid 250 and name CA) (segid 3A4 and resid 390 and name CA)	14.37	0.36	0.35

	assign (segid 3A4 and resid 250 and name CA)	(segid 3A4 and resid 390 and name CB)	15.64	0.35	0.36
	assign (segid 3A4 and resid 250 and name CA)	(segid 3A4 and resid 391 and name CA)	11.87	0.36	0.36
	assign (segid 3A4 and resid 250 and name CA)	(segid 3A4 and resid 391 and name CB)	12.21	0.35	0.34
	assign (segid 3A4 and resid 250 and name CA)	(segid 3A4 and resid 392 and name CA)	11.19	0.39	0.39
	assign (segid 3A4 and resid 250 and name CA)	(segid 3A4 and resid 392 and name CB)	10.15	0.47	0.46
5	assign (segid 3A4 and resid 250 and name CA)	(segid 3A4 and resid 393 and name CA)	11.20	0.33	0.32
	assign (segid 3A4 and resid 250 and name CA)	(segid 3A4 and resid 394 and name CA)	14.48	0.31	0.31
	assign (segid 3A4 and resid 250 and name CA)	(segid 3A4 and resid 394 and name CB)	15.26	0.34	0.33
	assign (segid 3A4 and resid 250 and name CA)	(segid 3A4 and resid 395 and name CA)	16.67	0.33	0.33
	assign (segid 3A4 and resid 250 and name CA)	(segid 3A4 and resid 396 and name CA)	15.02	0.32	0.32
10	assign (segid 3A4 and resid 250 and name CA)	(segid 3A4 and resid 396 and name CB)	13.76	0.39	0.39
	assign (segid 3A4 and resid 250 and name CA)	(segid 3A4 and resid 397 and name CA)	14.92	0.32	0.32
	assign (segid 3A4 and resid 250 and name CA)	(segid 3A4 and resid 397 and name CB)	14.32	0.32	0.33
	assign (segid 3A4 and resid 250 and name CA)	(segid 3A4 and resid 398 and name CA)	18.57	0.33	0.32
	assign (segid 3A4 and resid 250 and name CA)	(segid 3A4 and resid 398 and name CB)	19.18	0.32	0.33
15	assign (segid 3A4 and resid 250 and name CA)	(segid 3A4 and resid 399 and name CB)	19.27	0.31	0.31
	assign (segid 3A4 and resid 250 and name CA)	(segid 3A4 and resid 400 and name CA)	18.46	0.37	0.37
	assign (segid 3A4 and resid 250 and name CA)	(segid 3A4 and resid 400 and name CB)	17.07	0.40	0.40
	assign (segid 3A4 and resid 250 and name CA)	(segid HEM and resid 1 and name C1D)	7.30	0.30	0.30
20	assign (segid 3A4 and resid 250 and name CA)	(segid HEM and resid 1 and name C2D)	6.81	0.36	0.36
	assign (segid 3A4 and resid 250 and name CA)	(segid HEM and resid 1 and name CHD)	7.14	0.23	0.23
	assign (segid 3A4 and resid 250 and name CA)	(segid HEM and resid 1 and name CMD)	5.98	0.40	0.39
	assign (segid 3A4 and resid 250 and name CB)	(segid 3A4 and resid 251 and name C)	5.43	0.01	0.02
	assign (segid 3A4 and resid 250 and name CB)	(segid 3A4 and resid 251 and name CA)	4.50	0.05	0.04
	assign (segid 3A4 and resid 250 and name CB)	(segid 3A4 and resid 251 and name CB)	5.37	0.10	0.09
25	assign (segid 3A4 and resid 250 and name CB)	(segid 3A4 and resid 251 and name CG)	5.33	0.17	0.16
	assign (segid 3A4 and resid 250 and name CB)	(segid 3A4 and resid 251 and name N)	3.19	0.06	0.05
	assign (segid 3A4 and resid 250 and name CB)	(segid 3A4 and resid 251 and name O)	6.27	0.10	0.10
	assign (segid 3A4 and resid 250 and name CB)	(segid 3A4 and resid 252 and name C)	6.87	0.07	0.07
	assign (segid 3A4 and resid 250 and name CB)	(segid 3A4 and resid 252 and name CA)	6.81	0.07	0.08
30	assign (segid 3A4 and resid 250 and name CB)	(segid 3A4 and resid 252 and name CB)	7.25	0.09	0.10
	assign (segid 3A4 and resid 250 and name CB)	(segid 3A4 and resid 252 and name N)	5.64	0.10	0.10
	assign (segid 3A4 and resid 250 and name CB)	(segid 3A4 and resid 253 and name C)	6.75	0.14	0.13
	assign (segid 3A4 and resid 250 and name CB)	(segid 3A4 and resid 253 and name CA)	6.60	0.17	0.16
	assign (segid 3A4 and resid 250 and name CB)	(segid 3A4 and resid 253 and name N)	6.07	0.08	0.08
35	assign (segid 3A4 and resid 250 and name CB)	(segid 3A4 and resid 254 and name CA)	6.41	0.19	0.19
	assign (segid 3A4 and resid 250 and name CB)	(segid 3A4 and resid 254 and name N)	5.85	0.16	0.17
	assign (segid 3A4 and resid 250 and name CB)	(segid 3A4 and resid 255 and name CA)	8.89	0.42	0.41
	assign (segid 3A4 and resid 250 and name CB)	(segid 3A4 and resid 256 and name CA)	11.15	0.21	0.21
40	assign (segid 3A4 and resid 250 and name CB)	(segid 3A4 and resid 257 and name CA)	12.50	0.73	0.74
	assign (segid 3A4 and resid 250 and name CB)	(segid 3A4 and resid 258 and name CA)	13.10	0.63	0.62
	assign (segid 3A4 and resid 250 and name CB)	(segid 3A4 and resid 258 and name CB)	12.19	0.63	0.62
	assign (segid 3A4 and resid 250 and name CB)	(segid 3A4 and resid 259 and name CA)	14.91	0.33	0.33
	assign (segid 3A4 and resid 250 and name CB)	(segid 3A4 and resid 259 and name CB)	14.48	0.31	0.32
	assign (segid 3A4 and resid 250 and name CB)	(segid 3A4 and resid 260 and name CA)	16.88	0.44	0.44
45	assign (segid 3A4 and resid 250 and name CB)	(segid 3A4 and resid 260 and name CB)	16.50	0.52	0.52
	assign (segid 3A4 and resid 250 and name CB)	(segid 3A4 and resid 261 and name CA)	18.06	0.60	0.60
	assign (segid 3A4 and resid 250 and name CB)	(segid 3A4 and resid 262 and name CB)	18.30	0.38	0.38
	assign (segid 3A4 and resid 250 and name CB)	(segid 3A4 and resid 318 and name CA)	17.36	0.62	0.62
50	assign (segid 3A4 and resid 250 and name CB)	(segid 3A4 and resid 318 and name CB)	16.83	0.76	0.75
	assign (segid 3A4 and resid 250 and name CB)	(segid 3A4 and resid 319 and name CA)	15.14	0.63	0.63
	assign (segid 3A4 and resid 250 and name CB)	(segid 3A4 and resid 319 and name CB)	13.99	0.52	0.53
	assign (segid 3A4 and resid 250 and name CB)	(segid 3A4 and resid 322 and name CA)	15.92	0.97	0.96
	assign (segid 3A4 and resid 250 and name CB)	(segid 3A4 and resid 323 and name CA)	17.23	1.16	1.16
	assign (segid 3A4 and resid 250 and name CB)	(segid 3A4 and resid 383 and name CA)	17.95	0.54	0.54
55	assign (segid 3A4 and resid 250 and name CB)	(segid 3A4 and resid 384 and name CA)	15.17	0.39	0.38
	assign (segid 3A4 and resid 250 and name CB)	(segid 3A4 and resid 384 and name CB)	15.36	0.34	0.35
	assign (segid 3A4 and resid 250 and name CB)	(segid 3A4 and resid 385 and name CA)	15.60	0.54	0.54
	assign (segid 3A4 and resid 250 and name CB)	(segid 3A4 and resid 386 and name CA)	17.58	0.42	0.41
	assign (segid 3A4 and resid 250 and name CB)	(segid 3A4 and resid 387 and name CA)	17.60	0.47	0.48
60	assign (segid 3A4 and resid 250 and name CB)	(segid 3A4 and resid 388 and name CA)	15.49	0.36	0.36
	assign (segid 3A4 and resid 250 and name CB)	(segid 3A4 and resid 388 and name CB)	15.81	0.44	0.44
	assign (segid 3A4 and resid 250 and name CB)	(segid 3A4 and resid 389 and name CA)	12.33	0.49	0.49
	assign (segid 3A4 and resid 250 and name CB)	(segid 3A4 and resid 389 and name CB)	12.12	0.68	0.68
65	assign (segid 3A4 and resid 250 and name CB)	(segid 3A4 and resid 390 and name CA)	13.50	0.38	0.38
	assign (segid 3A4 and resid 250 and name CB)	(segid 3A4 and resid 390 and name CB)	14.78	0.37	0.38
	assign (segid 3A4 and resid 250 and name CB)	(segid 3A4 and resid 391 and name CA)	11.29	0.36	0.35
	assign (segid 3A4 and resid 250 and name CB)	(segid 3A4 and resid 391 and name CB)	11.79	0.34	0.34
	assign (segid 3A4 and resid 250 and name CB)	(segid 3A4 and resid 392 and name CA)	10.55	0.36	0.37
70	assign (segid 3A4 and resid 250 and name CB)	(segid 3A4 and resid 392 and name CB)	9.42	0.42	0.43
	assign (segid 3A4 and resid 250 and name CB)	(segid 3A4 and resid 393 and name CA)	11.06	0.34	0.34
	assign (segid 3A4 and resid 250 and name CB)	(segid 3A4 and resid 394 and name CA)	14.31	0.31	0.32
	assign (segid 3A4 and resid 250 and name CB)	(segid 3A4 and resid 394 and name CB)	14.97	0.34	0.34
	assign (segid 3A4 and resid 250 and name CB)	(segid 3A4 and resid 395 and name CA)	16.58	0.34	0.35
	assign (segid 3A4 and resid 250 and name CB)	(segid 3A4 and resid 396 and name CA)	15.23	0.36	0.36
75	assign (segid 3A4 and resid 250 and name CB)	(segid 3A4 and resid 396 and name CB)	14.00	0.45	0.45
	assign (segid 3A4 and resid 250 and name CB)	(segid 3A4 and resid 397 and name CA)	15.26	0.30	0.30
	assign (segid 3A4 and resid 250 and name CB)	(segid 3A4 and resid 397 and name CB)	14.60	0.30	0.31
	assign (segid 3A4 and resid 250 and name CB)	(segid 3A4 and resid 398 and name CA)	18.79	0.31	0.31
80	assign (segid 3A4 and resid 250 and name CB)	(segid 3A4 and resid 400 and name CA)	19.06	0.35	0.35
	assign (segid 3A4 and resid 250 and name CB)	(segid 3A4 and resid 400 and name CB)	17.72	0.38	0.39
	assign (segid 3A4 and resid 250 and name CB)	(segid HEM and resid 1 and name C1D)	6.97	0.27	0.27
	assign (segid 3A4 and resid 250 and name CB)	(segid HEM and resid 1 and name C2D)	6.21	0.31	0.31

5	assign (segid 3A4 and resid 250 and name CB)	(segid HEM and resid 1 and name C3D)	6.84	0.37	0.37
	assign (segid 3A4 and resid 250 and name CB)	(segid HEM and resid 1 and name CAD)	6.91	0.45	0.45
	assign (segid 3A4 and resid 250 and name CB)	(segid HEM and resid 1 and name CHD)	7.03	0.20	0.20
	assign (segid 3A4 and resid 250 and name CB)	(segid HEM and resid 1 and name CMD)	5.26	0.32	0.33
	assign (segid 3A4 and resid 250 and name N)	(segid 3A4 and resid 250 and name C)	2.45	0.03	0.03
	assign (segid 3A4 and resid 250 and name N)	(segid 3A4 and resid 250 and name CA)	1.45	0.00	0.01
	assign (segid 3A4 and resid 250 and name N)	(segid 3A4 and resid 250 and name CB)	2.45	0.03	0.03
	assign (segid 3A4 and resid 250 and name N)	(segid 3A4 and resid 250 and name O)	3.49	0.06	0.06
	assign (segid 3A4 and resid 250 and name N)	(segid 3A4 and resid 251 and name C)	4.73	0.07	0.06
10	assign (segid 3A4 and resid 250 and name N)	(segid 3A4 and resid 251 and name CA)	4.23	0.06	0.06
	assign (segid 3A4 and resid 250 and name N)	(segid 3A4 and resid 251 and name CB)	4.99	0.06	0.06
	assign (segid 3A4 and resid 250 and name N)	(segid 3A4 and resid 251 and name CG)	5.46	0.06	0.05
	assign (segid 3A4 and resid 250 and name N)	(segid 3A4 and resid 251 and name N)	2.82	0.06	0.06
	assign (segid 3A4 and resid 250 and name N)	(segid 3A4 and resid 251 and name O)	5.79	0.11	0.12
15	assign (segid 3A4 and resid 250 and name N)	(segid 3A4 and resid 252 and name C)	5.65	0.08	0.07
	assign (segid 3A4 and resid 250 and name N)	(segid 3A4 and resid 252 and name CA)	5.35	0.08	0.09
	assign (segid 3A4 and resid 250 and name N)	(segid 3A4 and resid 252 and name CB)	5.37	0.11	0.11
	assign (segid 3A4 and resid 250 and name N)	(segid 3A4 and resid 252 and name N)	4.36	0.11	0.12
	assign (segid 3A4 and resid 250 and name N)	(segid 3A4 and resid 252 and name O)	6.82	0.10	0.10
20	assign (segid 3A4 and resid 250 and name N)	(segid 3A4 and resid 253 and name C)	6.38	0.14	0.13
	assign (segid 3A4 and resid 250 and name N)	(segid 3A4 and resid 253 and name CA)	5.71	0.14	0.14
	assign (segid 3A4 and resid 250 and name N)	(segid 3A4 and resid 253 and name N)	4.88	0.09	0.08
	assign (segid 3A4 and resid 250 and name N)	(segid 3A4 and resid 253 and name O)	7.60	0.14	0.13
	assign (segid 3A4 and resid 250 and name N)	(segid 3A4 and resid 254 and name CA)	6.86	0.17	0.17
25	assign (segid 3A4 and resid 250 and name N)	(segid 3A4 and resid 254 and name N)	5.85	0.15	0.15
	assign (segid 3A4 and resid 250 and name N)	(segid HEM and resid 1 and name CMD)	7.15	0.38	0.37
	assign (segid 3A4 and resid 250 and name O)	(segid 3A4 and resid 250 and name CB)	3.27	0.04	0.03
	assign (segid 3A4 and resid 250 and name O)	(segid 3A4 and resid 251 and name C)	2.94	0.05	0.05
	assign (segid 3A4 and resid 250 and name O)	(segid 3A4 and resid 251 and name CA)	2.73	0.04	0.05
30	assign (segid 3A4 and resid 250 and name O)	(segid 3A4 and resid 251 and name CB)	4.22	0.05	0.05
	assign (segid 3A4 and resid 250 and name O)	(segid 3A4 and resid 251 and name CG)	4.91	0.08	0.07
	assign (segid 3A4 and resid 250 and name O)	(segid 3A4 and resid 251 and name N)	2.23	0.03	0.03
	assign (segid 3A4 and resid 250 and name O)	(segid 3A4 and resid 251 and name O)	3.40	0.17	0.16
	assign (segid 3A4 and resid 250 and name O)	(segid 3A4 and resid 252 and name C)	4.10	0.05	0.04
35	assign (segid 3A4 and resid 250 and name O)	(segid 3A4 and resid 252 and name CA)	4.37	0.09	0.09
	assign (segid 3A4 and resid 250 and name O)	(segid 3A4 and resid 252 and name CB)	5.31	0.10	0.10
	assign (segid 3A4 and resid 250 and name O)	(segid 3A4 and resid 252 and name N)	3.41	0.11	0.12
	assign (segid 3A4 and resid 250 and name O)	(segid 3A4 and resid 252 and name O)	4.88	0.08	0.08
40	assign (segid 3A4 and resid 250 and name O)	(segid 3A4 and resid 253 and name C)	3.90	0.03	0.04
	assign (segid 3A4 and resid 250 and name O)	(segid 3A4 and resid 253 and name CA)	4.05	0.07	0.07
	assign (segid 3A4 and resid 250 and name O)	(segid 3A4 and resid 253 and name N)	3.51	0.09	0.08
	assign (segid 3A4 and resid 250 and name O)	(segid 3A4 and resid 253 and name O)	5.05	0.04	0.04
	assign (segid 3A4 and resid 250 and name O)	(segid 3A4 and resid 254 and name C)	4.54	0.23	0.24
	assign (segid 3A4 and resid 250 and name O)	(segid 3A4 and resid 254 and name CA)	3.59	0.10	0.09
45	assign (segid 3A4 and resid 250 and name O)	(segid 3A4 and resid 254 and name N)	2.90	0.06	0.06
	assign (segid 3A4 and resid 250 and name O)	(segid 3A4 and resid 254 and name O)	5.68	0.23	0.23
	assign (segid 3A4 and resid 250 and name O)	(segid 3			

	assign (segid 3A4 and resid 251 and name C) (segid 3A4 and resid 255 and name N)	4.16	0.55	0.56
	assign (segid 3A4 and resid 251 and name C) (segid 3A4 and resid 256 and name CA)	6.90	0.34	0.35
	assign (segid 3A4 and resid 251 and name C) (segid 3A4 and resid 256 and name N)	5.77	0.41	0.40
	assign (segid 3A4 and resid 251 and name C) (segid HEM and resid 1 and name C1C)	7.45	0.31	0.31
5	assign (segid 3A4 and resid 251 and name C) (segid HEM and resid 1 and name C1D)	6.84	0.37	0.37
	assign (segid 3A4 and resid 251 and name C) (segid HEM and resid 1 and name C2C)	6.59	0.31	0.32
	assign (segid 3A4 and resid 251 and name C) (segid HEM and resid 1 and name C2D)	7.09	0.39	0.38
	assign (segid 3A4 and resid 251 and name C) (segid HEM and resid 1 and name C3C)	5.67	0.34	0.35
	assign (segid 3A4 and resid 251 and name C) (segid HEM and resid 1 and name C4C)	6.14	0.34	0.34
	assign (segid 3A4 and resid 251 and name C) (segid HEM and resid 1 and name CAC)	4.78	0.38	0.38
10	assign (segid 3A4 and resid 251 and name C) (segid HEM and resid 1 and name CBC)	4.85	0.32	0.32
	assign (segid 3A4 and resid 251 and name C) (segid HEM and resid 1 and name CHD)	5.89	0.37	0.37
	assign (segid 3A4 and resid 251 and name C) (segid HEM and resid 1 and name CMC)	7.08	0.34	0.35
	assign (segid 3A4 and resid 251 and name C) (segid HEM and resid 1 and name CMD)	6.45	0.40	0.41
	assign (segid 3A4 and resid 251 and name C) (segid HEM and resid 1 and name NC)	7.24	0.34	0.33
15	assign (segid 3A4 and resid 251 and name C) (segid HEM and resid 1 and name NC)	1.53	0.01	0.00
	assign (segid 3A4 and resid 251 and name CA) (segid 3A4 and resid 251 and name CB)	1.53	0.01	0.01
	assign (segid 3A4 and resid 251 and name CA) (segid 3A4 and resid 251 and name CG)	2.58	0.04	0.04
	assign (segid 3A4 and resid 251 and name CA) (segid 3A4 and resid 251 and name O)	2.40	0.03	0.02
	assign (segid 3A4 and resid 251 and name CA) (segid 3A4 and resid 252 and name C)	4.43	0.05	0.04
20	assign (segid 3A4 and resid 251 and name CA) (segid 3A4 and resid 252 and name CA)	3.81	0.01	0.01
	assign (segid 3A4 and resid 251 and name CA) (segid 3A4 and resid 252 and name CB)	4.83	0.03	0.02
	assign (segid 3A4 and resid 251 and name CA) (segid 3A4 and resid 252 and name N)	2.43	0.01	0.01
	assign (segid 3A4 and resid 251 and name CA) (segid 3A4 and resid 252 and name O)	5.20	0.09	0.10
	assign (segid 3A4 and resid 251 and name CA) (segid 3A4 and resid 253 and name C)	5.70	0.11	0.11
25	assign (segid 3A4 and resid 251 and name CA) (segid 3A4 and resid 253 and name CA)	5.68	0.08	0.09
	assign (segid 3A4 and resid 251 and name CA) (segid 3A4 and resid 253 and name N)	4.58	0.07	0.06
	assign (segid 3A4 and resid 251 and name CA) (segid 3A4 and resid 253 and name O)	6.78	0.13	0.12
	assign (segid 3A4 and resid 251 and name CA) (segid 3A4 and resid 254 and name C)	5.69	0.35	0.36
	assign (segid 3A4 and resid 251 and name CA) (segid 3A4 and resid 254 and name CA)	5.37	0.17	0.17
30	assign (segid 3A4 and resid 251 and name CA) (segid 3A4 and resid 254 and name N)	4.82	0.13	0.14
	assign (segid 3A4 and resid 251 and name CA) (segid 3A4 and resid 254 and name O)	6.81	0.39	0.39
	assign (segid 3A4 and resid 251 and name CA) (segid 3A4 and resid 255 and name CA)	5.80	0.68	0.68
	assign (segid 3A4 and resid 251 and name CA) (segid 3A4 and resid 255 and name N)	5.02	0.50	0.51
	assign (segid 3A4 and resid 251 and name CA) (segid 3A4 and resid 256 and name CA)	8.26	0.31	0.31
35	assign (segid 3A4 and resid 251 and name CA) (segid 3A4 and resid 256 and name N)	7.04	0.36	0.37
	assign (segid 3A4 and resid 251 and name CA) (segid 3A4 and resid 257 and name CA)	10.71	0.52	0.52
	assign (segid 3A4 and resid 251 and name CA) (segid 3A4 and resid 258 and name CA)	11.34	0.47	0.48
	assign (segid 3A4 and resid 251 and name CA) (segid 3A4 and resid 258 and name CB)	10.57	0.54	0.55
	assign (segid 3A4 and resid 251 and name CA) (segid 3A4 and resid 259 and name CA)	12.12	0.41	0.41
40	assign (segid 3A4 and resid 251 and name CA) (segid 3A4 and resid 259 and name CB)	11.36	0.49	0.49
	assign (segid 3A4 and resid 251 and name CA) (segid 3A4 and resid 260 and name CA)	14.18	0.40	0.39
	assign (segid 3A4 and resid 251 and name CA) (segid 3A4 and resid 260 and name CB)	13.90	0.45	0.46
	assign (segid 3A4 and resid 251 and name CA) (segid 3A4 and resid 261 and name CA)	16.10	0.45	0.45
	assign (segid 3A4 and resid 251 and name CA) (segid 3A4 and resid 262 and name CA)	16.82	0.32	0.32
45	assign (segid 3A4 and resid 251 and name CA) (segid 3A4 and resid 262 and name CB)	15.97	0.29	0.29
	assign (segid 3A4 and resid 251 and name CA) (segid 3A4 and resid 263 and name CA)	18.26	0.34	0.35
	assign (segid 3A4 and resid 251 and name CA) (segid 3A4 and resid 263 and name CB)	17.66	0.38	0.37
	assign (segid 3A4 and resid 251 and name CA) (segid 3A4 and resid 313 and name CB)	18.75	0.60	0.59
	assign (segid 3A4 and resid 251 and name CA) (segid 3A4 and resid 318 and name CA)	16.74	0.65	0.64
50	assign (segid 3A4 and resid 251 and name CA) (segid 3A4 and resid 318 and name CB)	15.88	0.75	0.74
	assign (segid 3A4 and resid 251 and name CA) (segid 3A4 and resid 319 and name CA)	15.38	0.64	0.64
	assign (segid 3A4 and resid 251 and name CA) (segid 3A4 and resid 319 and name CB)	14.24	0.61	0.62
	assign (segid 3A4 and resid 251 and name CA) (segid 3A4 and resid 322 and name CA)	18.76	0.65	0.65
	assign (segid 3A4 and resid 251 and name CA) (segid 3A4 and resid 383 and name CA)	17.41	0.24	0.24
55	assign (segid 3A4 and resid 251 and name CA) (segid 3A4 and resid 384 and name CA)	14.60	0.27	0.26
	assign (segid 3A4 and resid 251 and name CA) (segid 3A4 and resid 384 and name CB)	14.47	0.37	0.37
	assign (segid 3A4 and resid 251 and name CA) (segid 3A4 and resid 385 and name CA)	16.06	0.15	0.16
	assign (segid 3A4 and resid 251 and name CA) (segid 3A4 and resid 386 and name CA)	18.28	0.22	0.22
	assign (segid 3A4 and resid 251 and name CA) (segid 3A4 and resid 387 and name CA)	18.75	0.37	0.37
60	assign (segid 3A4 and resid 251 and name CA) (segid 3A4 and resid 388 and name CA)	16.89	0.18	0.18
	assign (segid 3A4 and resid 251 and name CA) (segid 3A4 and resid 388 and name CB)	17.51	0.22	0.22
	assign (segid 3A4 and resid 251 and name CA) (segid 3A4 and resid 389 and name CA)	13.89	0.31	0.31
	assign (segid 3A4 and resid 251 and name CA) (segid 3A4 and resid 389 and name CB)	14.06	0.48	0.48
	assign (segid 3A4 and resid 251 and name CA) (segid 3A4 and resid 390 and name CA)	13.91	0.28	0.28
65	assign (segid 3A4 and resid 251 and name CA) (segid 3A4 and resid 390 and name CB)	14.96	0.31	0.32
	assign (segid 3A4 and resid 251 and name CA) (segid 3A4 and resid 391 and name CA)	10.80	0.35	0.35
	assign (segid 3A4 and resid 251 and name CA) (segid 3A4 and resid 391 and name CB)	10.95	0.38	0.38
	assign (segid 3A4 and resid 251 and name CA) (segid 3A4 and resid 392 and name CA)	9.40	0.46	0.46
	assign (segid 3A4 and resid 251 and name CA) (segid 3A4 and resid 392 and name CB)	8.48	0.53	0.53
70	assign (segid 3A4 and resid 251 and name CA) (segid 3A4 and resid 393 and name CA)	8.53	0.36	0.35
	assign (segid 3A4 and resid 251 and name CA) (segid 3A4 and resid 394 and name CA)	12.09	0.35	0.36
	assign (segid 3A4 and resid 251 and name CA) (segid 3A4 and resid 394 and name CB)	13.10	0.35	0.34
	assign (segid 3A4 and resid 251 and name CA) (segid 3A4 and resid 395 and name CA)	13.71	0.37	0.37
	assign (segid 3A4 and resid 251 and name CA) (segid 3A4 and resid 396 and name CA)	11.67	0.41	0.40
75	assign (segid 3A4 and resid 251 and name CA) (segid 3A4 and resid 396 and name CB)	10.31	0.43	0.44
	assign (segid 3A4 and resid 251 and name CA) (segid 3A4 and resid 397 and name CA)	12.02	0.52	0.51
	assign (segid 3A4 and resid 251 and name CA) (segid 3A4 and resid 397 and name CB)	11.69	0.52	0.52
	assign (segid 3A4 and resid 251 and name CA) (segid 3A4 and resid 398 and name CA)	15.69	0.49	0.49
	assign (segid 3A4 and resid 251 and name CA) (segid 3A4 and resid 398 and name CB)	16.37	0.48	0.48
80	assign (segid 3A4 and resid 251 and name CA) (segid 3A4 and resid 399 and name CA)	16.34	0.44	0.44
	assign (segid 3A4 and resid 251 and name CA) (segid 3A4 and resid 399 and name CB)	15.84	0.43	0.43
	assign (segid 3A4 and resid 251 and name CA) (segid 3A4 and resid 400 and name CA)	15.21	0.54	0.53

	assign (segid 3A4 and resid 251 and name CA)	(segid 3A4 and resid 400 and name CB)	13.86	0.57	0.57
	assign (segid 3A4 and resid 251 and name CA)	(segid 3A4 and resid 401 and name CA)	17.25	0.66	0.66
	assign (segid 3A4 and resid 251 and name CA)	(segid HEM and resid 1 and name C1C)	7.61	0.27	0.27
	assign (segid 3A4 and resid 251 and name CA)	(segid HEM and resid 1 and name C1D)	6.22	0.32	0.32
5	assign (segid 3A4 and resid 251 and name CA)	(segid HEM and resid 1 and name C2C)	6.82	0.27	0.28
	assign (segid 3A4 and resid 251 and name CA)	(segid HEM and resid 1 and name C2D)	6.21	0.34	0.35
	assign (segid 3A4 and resid 251 and name CA)	(segid HEM and resid 1 and name C3C)	5.68	0.29	0.30
	assign (segid 3A4 and resid 251 and name CA)	(segid HEM and resid 1 and name C3D)	7.43	0.33	0.33
	assign (segid 3A4 and resid 251 and name CA)	(segid HEM and resid 1 and name C4C)	5.96	0.28	0.27
10	assign (segid 3A4 and resid 251 and name CA)	(segid HEM and resid 1 and name CAC)	4.71	0.31	0.31
	assign (segid 3A4 and resid 251 and name CA)	(segid HEM and resid 1 and name CBC)	4.84	0.32	0.33
	assign (segid 3A4 and resid 251 and name CA)	(segid HEM and resid 1 and name CHD)	5.40	0.31	0.31
	assign (segid 3A4 and resid 251 and name CA)	(segid HEM and resid 1 and name CMD)	5.34	0.36	0.37
	assign (segid 3A4 and resid 251 and name CA)	(segid HEM and resid 1 and name NC)	7.18	0.28	0.28
15	assign (segid 3A4 and resid 251 and name CA)	(segid HEM and resid 1 and name ND)	7.43	0.31	0.30
	assign (segid 3A4 and resid 251 and name CB)	(segid 3A4 and resid 251 and name CG)	1.53	0.00	0.01
	assign (segid 3A4 and resid 251 and name CB)	(segid 3A4 and resid 252 and name C)	5.48	0.08	0.08
	assign (segid 3A4 and resid 251 and name CB)	(segid 3A4 and resid 252 and name CA)	4.51	0.05	0.05
	assign (segid 3A4 and resid 251 and name CB)	(segid 3A4 and resid 252 and name CB)	5.34	0.05	0.05
20	assign (segid 3A4 and resid 251 and name CB)	(segid 3A4 and resid 252 and name N)	3.18	0.07	0.07
	assign (segid 3A4 and resid 251 and name CB)	(segid 3A4 and resid 252 and name O)	6.23	0.11	0.11
	assign (segid 3A4 and resid 251 and name CB)	(segid 3A4 and resid 253 and name C)	7.14	0.12	0.12
	assign (segid 3A4 and resid 251 and name CB)	(segid 3A4 and resid 253 and name CA)	7.04	0.09	0.09
	assign (segid 3A4 and resid 251 and name CB)	(segid 3A4 and resid 253 and name N)	5.81	0.08	0.08
25	assign (segid 3A4 and resid 251 and name CB)	(segid 3A4 and resid 254 and name CA)	6.81	0.20	0.20
	assign (segid 3A4 and resid 251 and name CB)	(segid 3A4 and resid 254 and name N)	6.31	0.15	0.15
	assign (segid 3A4 and resid 251 and name CB)	(segid 3A4 and resid 255 and name CA)	6.73	0.77	0.77
	assign (segid 3A4 and resid 251 and name CB)	(segid 3A4 and resid 255 and name N)	6.19	0.55	0.55
	assign (segid 3A4 and resid 251 and name CB)	(segid 3A4 and resid 256 and name CA)	9.17	0.40	0.40
30	assign (segid 3A4 and resid 251 and name CB)	(segid 3A4 and resid 257 and name CA)	11.91	0.51	0.50
	assign (segid 3A4 and resid 251 and name CB)	(segid 3A4 and resid 258 and name CA)	12.50	0.49	0.49
	assign (segid 3A4 and resid 251 and name CB)	(segid 3A4 and resid 258 and name CB)	11.73	0.57	0.57
	assign (segid 3A4 and resid 251 and name CB)	(segid 3A4 and resid 259 and name CA)	12.93	0.51	0.52
	assign (segid 3A4 and resid 251 and name CB)	(segid 3A4 and resid 259 and name CB)	12.04	0.61	0.60
35	assign (segid 3A4 and resid 251 and name CB)	(segid 3A4 and resid 260 and name CA)	15.04	0.49	0.50
	assign (segid 3A4 and resid 251 and name CB)	(segid 3A4 and resid 260 and name CB)	14.80	0.54	0.54
	assign (segid 3A4 and resid 251 and name CB)	(segid 3A4 and resid 261 and name CA)	17.17	0.50	0.50
	assign (segid 3A4 and resid 251 and name CB)	(segid 3A4 and resid 262 and name CA)	17.73	0.41	0.41
	assign (segid 3A4 and resid 251 and name CB)	(segid 3A4 and resid 262 and name CB)	16.83	0.40	0.40
40	assign (segid 3A4 and resid 251 and name CB)	(segid 3A4 and resid 263 and name CA)	18.98	0.47	0.47
	assign (segid 3A4 and resid 251 and name CB)	(segid 3A4 and resid 263 and name CB)	18.31	0.51	0.51
	assign (segid 3A4 and resid 251 and name CB)	(segid 3A4 and resid 318 and name CA)	17.98	0.68	0.69
	assign (segid 3A4 and resid 251 and name CB)	(segid 3A4 and resid 318 and name CB)	17.08	0.79	0.79
	assign (segid 3A4 and resid 251 and name CB)	(segid 3A4 and resid 319 and name CA)	16.70	0.66	0.66
45	assign (segid 3A4 and resid 251 and name CB)	(segid 3A4 and resid 319 and name CB)	15.54	0.64	0.64
	assign (segid 3A4 and resid 251 and name CB)	(segid 3A4 and resid 383 and name CA)	18.34	0.25	0.24
	assign (segid 3A4 and resid 251 and name CB)	(segid 3A4 and resid 384 and name CA)	15.38	0.25	0.25
	assign (segid 3A4 and resid 251 and name CB)	(segid 3A4 and resid 384 and name CB)	15.12	0.37	0.38
	assign (segid 3A4 and resid 251 and name CB)	(segid 3A4 and resid 385 and name CA)	16.91	0.12	0.11
50	assign (segid 3A4 and resid 251 and name CB)	(segid 3A4 and resid 386 and name CA)	18.93	0.22	0.21
	assign (segid 3A4 and resid 251 and name CB)	(segid 3A4 and resid 387 and name CA)	19.23	0.35	0.35
	assign (segid 3A4 and resid 251 and name CB)	(segid 3A4 and resid 388 and name CA)	17.20	0.18	0.18
	assign (segid 3A4 and resid 251 and name CB)	(segid 3A4 and resid 388 and name CB)	17.79	0.22	0.21
	assign (segid 3A4 and resid 251 and name CB)	(segid 3A4 and resid 389 and name CA)	14.42	0.32	0.33
55	assign (segid 3A4 and resid 251 and name CB)	(segid 3A4 and resid 389 and name CB)	14.72	0.50	0.49
	assign (segid 3A4 and resid 251 and name CB)	(segid 3A4 and resid 390 and name CA)	14.43	0.25	0.25
	assign (segid 3A4 and resid 251 and name CB)	(segid 3A4 and resid 390 and name CB)	15.38	0.28	0.29
	assign (segid 3A4 and resid 251 and name CB)	(segid 3A4 and resid 391 and name CA)	11.34	0.33	0.33
	assign (segid 3A4 and resid 251 and name CB)	(segid 3A4 and resid 391 and name CB)	11.57	0.37	0.37
60	assign (segid 3A4 and resid 251 and name CB)	(segid 3A4 and resid 392 and name CA)	9.46	0.46	0.46
	assign (segid 3A4 and resid 251 and name CB)	(segid 3A4 and resid 392 and name CB)	8.45	0.52	0.52
	assign (segid 3A4 and resid 251 and name CB)	(segid 3A4 and resid 393 and name CA)	8.60	0.40	0.39
	assign (segid 3A4 and resid 251 and name CB)	(segid 3A4 and resid 394 and name CA)	12.31	0.39	0.40
	assign (segid 3A4 and resid 251 and name CB)	(segid 3A4 and resid 394 and name CB)	13.34	0.37	0.38
65	assign (segid 3A4 and resid 251 and name CB)	(segid 3A4 and resid 395 and name CA)	13.55	0.43	0.44
	assign (segid 3A4 and resid 251 and name CB)	(segid 3A4 and resid 396 and name CA)	11.44	0.53	0.52
	assign (segid 3A4 and resid 251 and name CB)	(segid 3A4 and resid 396 and name CB)	10.01	0.54	0.55
	assign (segid 3A4 and resid 251 and name CB)	(segid 3A4 and resid 397 and name CA)	12.26	0.65	0.64
	assign (segid 3A4 and resid 251 and name CB)	(segid 3A4 and resid 397 and name CB)	12.08	0.64	0.63
70	assign (segid 3A4 and resid 251 and name CB)	(segid 3A4 and resid 398 and name CA)	15.85	0.61	0.61
	assign (segid 3A4 and resid 251 and name CB)	(segid 3A4 and resid 398 and name CB)	16.50	0.58	0.59
	assign (segid 3A4 and resid 251 and name CB)	(segid 3A4 and resid 399 and name CA)	16.21	0.58	0.58
	assign (segid 3A4 and resid 251 and name CB)	(segid 3A4 and resid 399 and name CB)	15.58	0.56	0.56
	assign (segid 3A4 and resid 251 and name CB)	(segid 3A4 and resid 400 and name CA)	15.22	0.72	0.71
75	assign (segid 3A4 and resid 251 and name CB)	(segid 3A4 and resid 400 and name CB)	13.92	0.75	0.75
	assign (segid 3A4 and resid 251 and name CB)	(segid 3A4 and resid 401 and name CA)	17.53	0.81	0.81
	assign (segid 3A4 and resid 251 and name CB)	(segid HEM and resid 1 and name C1D)	7.02	0.26	0.26
	assign (segid 3A4 and resid 251 and name CB)	(segid HEM and resid 1 and name C2D)	6.95	0.28	0.27
	assign (segid 3A4 and resid 251 and name CB)	(segid HEM and resid 1 and name C3C)	6.24	0.35	0.36
80	assign (segid 3A4 and resid 251 and name CB)	(segid HEM and resid 1 and name C4C)	6.68	0.30	0.29
	assign (segid 3A4 and resid 251 and name CB)	(segid HEM and resid 1 and name CAC)	5.04	0.36	0.37
	assign (segid 3A4 and resid 251 and name CB)	(segid HEM and resid 1 and name CBC)	4.86	0.37	0.36
	assign (segid 3A4 and resid 251 and name CB)	(segid HEM and resid 1 and name CHD)	6.14	0.28	0.28

	assign (segid 3A4 and resid 252 and name C) (segid 3A4 and resid 254 and name C)	4.79	0.26	0.25
	assign (segid 3A4 and resid 252 and name C) (segid 3A4 and resid 254 and name CA)	4.66	0.11	0.11
	assign (segid 3A4 and resid 252 and name C) (segid 3A4 and resid 254 and name N)	3.44	0.10	0.10
	assign (segid 3A4 and resid 252 and name C) (segid 3A4 and resid 254 and name O)	5.87	0.27	0.27
	assign (segid 3A4 and resid 252 and name C) (segid 3A4 and resid 255 and name C)	5.00	0.39	0.39
5	assign (segid 3A4 and resid 252 and name C) (segid 3A4 and resid 255 and name CA)	4.79	0.49	0.48
	assign (segid 3A4 and resid 252 and name C) (segid 3A4 and resid 255 and name N)	4.04	0.35	0.36
	assign (segid 3A4 and resid 252 and name C) (segid 3A4 and resid 255 and name O)	6.12	0.38	0.39
	assign (segid 3A4 and resid 252 and name C) (segid 3A4 and resid 256 and name C)	6.24	0.33	0.34
	assign (segid 3A4 and resid 252 and name C) (segid 3A4 and resid 256 and name CA)	5.13	0.33	0.34
10	assign (segid 3A4 and resid 252 and name C) (segid 3A4 and resid 256 and name N)	4.33	0.35	0.35
	assign (segid 3A4 and resid 252 and name C) (segid 3A4 and resid 256 and name O)	7.34	0.33	0.34
	assign (segid 3A4 and resid 252 and name C) (segid 3A4 and resid 257 and name N)	6.20	0.40	0.39
	assign (segid 3A4 and resid 252 and name C) (segid HEM and resid 1 and name C3C)	7.25	0.35	0.34
	assign (segid 3A4 and resid 252 and name C) (segid HEM and resid 1 and name CAC)	6.75	0.41	0.40
15	assign (segid 3A4 and resid 252 and name C) (segid HEM and resid 1 and name CBC)	6.92	0.36	0.37
	assign (segid 3A4 and resid 252 and name CA) (segid 3A4 and resid 252 and name C)	1.53	0.02	0.01
	assign (segid 3A4 and resid 252 and name CA) (segid 3A4 and resid 252 and name CB)	1.52	0.01	0.01
	assign (segid 3A4 and resid 252 and name CA) (segid 3A4 and resid 252 and name O)	2.40	0.02	0.01
	assign (segid 3A4 and resid 252 and name CA) (segid 3A4 and resid 253 and name C)	4.51	0.07	0.08
20	assign (segid 3A4 and resid 252 and name CA) (segid 3A4 and resid 253 and name CA)	3.81	0.03	0.03
	assign (segid 3A4 and resid 252 and name CA) (segid 3A4 and resid 253 and name N)	2.44	0.03	0.03
	assign (segid 3A4 and resid 252 and name CA) (segid 3A4 and resid 253 and name O)	5.40	0.12	0.12
	assign (segid 3A4 and resid 252 and name CA) (segid 3A4 and resid 254 and name C)	5.79	0.30	0.30
	assign (segid 3A4 and resid 252 and name CA) (segid 3A4 and resid 254 and name CA)	5.72	0.14	0.14
25	assign (segid 3A4 and resid 252 and name CA) (segid 3A4 and resid 254 and name N)	4.58	0.12	0.13
	assign (segid 3A4 and resid 252 and name CA) (segid 3A4 and resid 254 and name O)	6.90	0.32	0.33
	assign (segid 3A4 and resid 252 and name CA) (segid 3A4 and resid 255 and name C)	5.76	0.50	0.51
	assign (segid 3A4 and resid 252 and name CA) (segid 3A4 and resid 255 and name CA)	5.43	0.63	0.63
	assign (segid 3A4 and resid 252 and name CA) (segid 3A4 and resid 255 and name N)	4.87	0.45	0.45
30	assign (segid 3A4 and resid 252 and name CA) (segid 3A4 and resid 255 and name O)	7.33	0.39	0.39
	assign (segid 3A4 and resid 252 and name CA) (segid 3A4 and resid 256 and name C)	6.07	0.43	0.42
	assign (segid 3A4 and resid 252 and name CA) (segid 3A4 and resid 256 and name N)	5.29	0.44	0.44
	assign (segid 3A4 and resid 252 and name CA) (segid 3A4 and resid 256 and name O)	8.80	0.42	0.42
	assign (segid 3A4 and resid 252 and name CA) (segid 3A4 and resid 257 and name CA)	10.62	0.38	0.38
35	assign (segid 3A4 and resid 252 and name CA) (segid 3A4 and resid 258 and name CA)	10.34	0.46	0.47
	assign (segid 3A4 and resid 252 and name CA) (segid 3A4 and resid 258 and name CB)	11.26	0.44	0.44
	assign (segid 3A4 and resid 252 and name CA) (segid 3A4 and resid 259 and name CA)	10.52	0.58	0.58
	assign (segid 3A4 and resid 252 and name CA) (segid 3A4 and resid 259 and name CB)	12.34	0.38	0.39
	assign (segid 3A4 and resid 252 and name CA) (segid 3A4 and resid 260 and name CA)	11.74	0.44	0.44
40	assign (segid 3A4 and resid 252 and name CA) (segid 3A4 and resid 260 and name CB)	14.61	0.46	0.45
	assign (segid 3A4 and resid 252 and name CA) (segid 3A4 and resid 261 and name CA)	16.00	0.35	0.35
	assign (segid 3A4 and resid 252 and name CA) (segid 3A4 and resid 262 and name CA)	15.43	0.33	0.33
	assign (segid 3A4 and resid 252 and name CA) (segid 3A4 and resid 262 and name CB)	17.01	0.41	0.41
	assign (segid 3A4 and resid 252 and name CA) (segid 3A4 and resid 263 and name CA)	16.24	0.45	0.44
45	assign (segid 3A4 and resid 252 and name CA) (segid 3A4 and resid 263 and name CB)	18.63	0.52	0.51
	assign (segid 3A4 and resid 252 and name CA) (segid 3A4 and resid 264 and name CA)	16.57	0.73	0.73
	assign (segid 3A4 and resid 252 and name CA) (segid 3A4 and resid 264 and name CB)	15.58	0.77	0.78
	assign (segid 3A4 and resid 252 and name CA) (segid 3A4 and resid 265 and name CA)	15.76	0.78	0.78
	assign (segid 3A4 and resid 252 and name CA) (segid 3A4 and resid 265 and name CB)	14.90	0.77	0.77
50	assign (segid 3A4 and resid 252 and name CA) (segid 3A4 and resid 266 and name CA)	18.74	0.26	0.26
	assign (segid 3A4 and resid 252 and name CA) (segid 3A4 and resid 266 and name CB)	16.49	0.32	0.33
	assign (segid 3A4 and resid 252 and name CA) (segid 3A4 and resid 267 and name CA)	16.48	0.45	0.45
	assign (segid 3A4 and resid 252 and name CA) (segid 3A4 and resid 267 and name CB)	18.29	0.23	0.23
	assign (segid 3A4 and resid 252 and name CA) (segid 3A4 and resid 268 and name CA)	17.08	0.28	0.28
55	assign (segid 3A4 and resid 252 and name CA) (segid 3A4 and resid 268 and name CB)	17.11	0.45	0.45
	assign (segid 3A4 and resid 252 and name CA) (segid 3A4 and resid 269 and name CA)	16.87	0.31	0.31
	assign (segid 3A4 and resid 252 and name CA) (segid 3A4 and resid 269 and name CB)	17.95	0.35	0.36
	assign (segid 3A4 and resid 252 and name CA) (segid 3A4 and resid 270 and name CA)	13.54	0.39	0.39
	assign (segid 3A4 and resid 252 and name CA) (segid 3A4 and resid 270 and name CB)	13.35	0.43	0.44
60	assign (segid 3A4 and resid 252 and name CA) (segid 3A4 and resid 271 and name CA)	12.62	0.47	0.48
	assign (segid 3A4 and resid 252 and name CA) (segid 3A4 and resid 271 and name CB)	11.93	0.55	0.55
	assign (segid 3A4 and resid 252 and name CA) (segid 3A4 and resid 272 and name CA)	10.94	0.36	0.36
	assign (segid 3A4 and resid 252 and name CA) (segid 3A4 and resid 272 and name CB)	14.16	0.37	0.36
	assign (segid 3A4 and resid 252 and name CA) (segid 3A4 and resid 273 and name CA)	15.34	0.36	0.36
65	assign (segid 3A4 and resid 252 and name CA) (segid 3A4 and resid 273 and name CB)	15.65	0.36	0.37
	assign (segid 3A4 and resid 252 and name CA) (segid 3A4 and resid 274 and name CA)	12.98	0.37	0.37
	assign (segid 3A4 and resid 252 and name CA) (segid 3A4 and resid 274 and name CB)	11.67	0.37	0.37
	assign (segid 3A4 and resid 252 and name CA) (segid 3A4 and resid 275 and name CA)	12.78	0.54	0.55
	assign (segid 3A4 and resid 252 and name CA) (segid 3A4 and resid 275 and name CB)	12.59	0.56	0.57
70	assign (segid 3A4 and resid 252 and name CA) (segid 3A4 and resid 276 and name CA)	16.58	0.55	0.54
	assign (segid 3A4 and resid 252 and name CA) (segid 3A4 and resid 276 and name CB)	17.53	0.54	0.53
	assign (segid 3A4 and resid 252 and name CA) (segid 3A4 and resid 277 and name CA)	16.98	0.49	0.50
	assign (segid 3A4 and resid 252 and name CA) (segid 3A4 and resid 277 and name CB)	16.62	0.51	0.50
	assign (segid 3A4 and resid 252 and name CA) (segid 3A4 and resid 278 and name CA)	15.03	0.58	0.58
75	assign (segid 3A4 and resid 252 and name CA) (segid 3A4 and resid 278 and name CB)	13.57	0.59	0.59
	assign (segid 3A4 and resid 252 and name CA) (segid 3A4 and resid 279 and name CA)	16.99	0.76	0.76
	assign (segid 3A4 and resid 252 and name CA) (segid 3A4 and resid 279 and name CB)	17.64	1.13	1.14
	assign (segid 3A4 and resid 252 and name CA) (segid 3A4 and resid 280 and name CA)	17.69	0.59	0.59
80	assign (segid 3A4 and resid 252 and name CA) (segid HEM and resid 1 and name CAC)	6.67	0.46	0.46
	assign (segid 3A4 and resid 252 and name CA) (segid HEM and resid 1 and name CBC)	6.64	0.30	0.29
	assign (segid 3A4 and resid 252 and name CB) (segid 3A4 and resid 253 and name C)	5.43	0.06	0.06
	assign (segid 3A4 and resid 252 and name CB) (segid 3A4 and resid 253 and name CA)	4.36	0.05	0.06

	assign (segid 3A4 and resid 252 and name CB)	(segid 3A4 and resid 253 and name N)	3.03	0.04	0.04
	assign (segid 3A4 and resid 252 and name CB)	(segid 3A4 and resid 253 and name O)	6.31	0.11	0.12
	assign (segid 3A4 and resid 252 and name CB)	(segid 3A4 and resid 254 and name C)	7.16	0.27	0.26
	assign (segid 3A4 and resid 252 and name CB)	(segid 3A4 and resid 254 and name CA)	6.96	0.10	0.10
5	assign (segid 3A4 and resid 252 and name CB)	(segid 3A4 and resid 254 and name N)	5.69	0.09	0.09
	assign (segid 3A4 and resid 252 and name CB)	(segid 3A4 and resid 255 and name CA)	6.88	0.61	0.60
	assign (segid 3A4 and resid 252 and name CB)	(segid 3A4 and resid 255 and name N)	6.31	0.42	0.42
	assign (segid 3A4 and resid 252 and name CB)	(segid 3A4 and resid 256 and name CA)	7.03	0.47	0.46
	assign (segid 3A4 and resid 252 and name CB)	(segid 3A4 and resid 256 and name N)	6.46	0.45	0.44
10	assign (segid 3A4 and resid 252 and name CB)	(segid 3A4 and resid 257 and name CA)	9.64	0.41	0.40
	assign (segid 3A4 and resid 252 and name CB)	(segid 3A4 and resid 258 and name CA)	11.80	0.35	0.36
	assign (segid 3A4 and resid 252 and name CB)	(segid 3A4 and resid 258 and name CB)	11.63	0.44	0.45
	assign (segid 3A4 and resid 252 and name CB)	(segid 3A4 and resid 259 and name CA)	12.48	0.46	0.46
	assign (segid 3A4 and resid 252 and name CB)	(segid 3A4 and resid 259 and name CB)	11.77	0.63	0.62
15	assign (segid 3A4 and resid 252 and name CB)	(segid 3A4 and resid 260 and name CA)	13.25	0.40	0.40
	assign (segid 3A4 and resid 252 and name CB)	(segid 3A4 and resid 260 and name CB)	12.52	0.44	0.43
	assign (segid 3A4 and resid 252 and name CB)	(segid 3A4 and resid 261 and name CA)	15.56	0.47	0.47
	assign (segid 3A4 and resid 252 and name CB)	(segid 3A4 and resid 262 and name CA)	17.17	0.36	0.36
	assign (segid 3A4 and resid 252 and name CB)	(segid 3A4 and resid 262 and name CB)	16.68	0.35	0.34
20	assign (segid 3A4 and resid 252 and name CB)	(segid 3A4 and resid 263 and name CA)	18.06	0.46	0.46
	assign (segid 3A4 and resid 252 and name CB)	(segid 3A4 and resid 263 and name CB)	17.24	0.50	0.51
	assign (segid 3A4 and resid 252 and name CB)	(segid 3A4 and resid 318 and name CA)	17.73	0.70	0.70
	assign (segid 3A4 and resid 252 and name CB)	(segid 3A4 and resid 318 and name CB)	16.75	0.75	0.75
	assign (segid 3A4 and resid 252 and name CB)	(segid 3A4 and resid 319 and name CA)	16.89	0.75	0.76
25	assign (segid 3A4 and resid 252 and name CB)	(segid 3A4 and resid 319 and name CB)	16.09	0.74	0.74
	assign (segid 3A4 and resid 252 and name CB)	(segid 3A4 and resid 384 and name CA)	17.94	0.31	0.31
	assign (segid 3A4 and resid 252 and name CB)	(segid 3A4 and resid 384 and name CB)	17.96	0.43	0.43
	assign (segid 3A4 and resid 252 and name CB)	(segid 3A4 and resid 389 and name CA)	18.22	0.32	0.33
	assign (segid 3A4 and resid 252 and name CB)	(segid 3A4 and resid 389 and name CB)	18.20	0.51	0.51
30	assign (segid 3A4 and resid 252 and name CB)	(segid 3A4 and resid 390 and name CA)	18.20	0.28	0.29
	assign (segid 3A4 and resid 252 and name CB)	(segid 3A4 and resid 391 and name CA)	14.95	0.38	0.37
	assign (segid 3A4 and resid 252 and name CB)	(segid 3A4 and resid 391 and name CB)	14.81	0.42	0.42
	assign (segid 3A4 and resid 252 and name CB)	(segid 3A4 and resid 392 and name CA)	13.97	0.47	0.47
	assign (segid 3A4 and resid 252 and name CB)	(segid 3A4 and resid 392 and name CB)	13.19	0.54	0.54
35	assign (segid 3A4 and resid 252 and name CB)	(segid 3A4 and resid 393 and name CA)	12.39	0.38	0.37
	assign (segid 3A4 and resid 252 and name CB)	(segid 3A4 and resid 394 and name CA)	15.66	0.38	0.37
	assign (segid 3A4 and resid 252 and name CB)	(segid 3A4 and resid 394 and name CB)	16.84	0.37	0.36
	assign (segid 3A4 and resid 252 and name CB)	(segid 3A4 and resid 395 and name CA)	17.08	0.39	0.39
	assign (segid 3A4 and resid 252 and name CB)	(segid 3A4 and resid 396 and name CA)	14.33	0.43	0.42
40	assign (segid 3A4 and resid 252 and name CB)	(segid 3A4 and resid 396 and name CB)	12.99	0.41	0.42
	assign (segid 3A4 and resid 252 and name CB)	(segid 3A4 and resid 397 and name CA)	14.21	0.58	0.58
	assign (segid 3A4 and resid 252 and name CB)	(segid 3A4 and resid 397 and name CB)	14.06	0.58	0.59
	assign (segid 3A4 and resid 252 and name CB)	(segid 3A4 and resid 398 and name CA)	18.00	0.59	0.58
	assign (segid 3A4 and resid 252 and name CB)	(segid 3A4 and resid 399 and name CA)	18.27	0.56	0.57
45	assign (segid 3A4 and resid 252 and name CB)	(segid 3A4 and resid 399 and name CB)	17.88	0.58	0.57
	assign (segid 3A4 and resid 252 and name CB)	(segid 3A4 and resid 400 and name CA)	16.21	0.66	0.67
	assign (segid 3A4 and resid 252 and name CB)	(segid 3A4 and resid 400 and name CB)	14.75	0.68	0.68
	assign (segid 3A4 and resid 252 and name CB)	(segid 3A4 and resid 401 and name CA)	18.23	0.83	0.83
	assign (segid 3A4 and resid 252 and name CB)	(segid 3A4 and resid 434 and name CA)	18.49	0.61	0.61
50	assign (segid 3A4 and resid 252 and name CB)	(segid 3A4 and resid 252 and name C)	2.45	0.02	0.02
	assign (segid 3A4 and resid 252 and name N)	(segid 3A4 and resid 252 and name CA)	1.46	0.01	0.00
	assign (segid 3A4 and resid 252 and name N)	(segid 3A4 and resid 252 and name CB)	2.43	0.02	0.02
	assign (segid 3A4 and resid 252 and name N)	(segid 3A4 and resid 252 and name O)	3.43	0.04	0.03
	assign (segid 3A4 and resid 252 and name N)	(segid 3A4 and resid 253 and name C)	4.81	0.07	0.07
55	assign (segid 3A4 and resid 252 and name N)	(segid 3A4 and resid 253 and name CA)	4.29	0.04	0.05
	assign (segid 3A4 and resid 252 and name N)	(segid 3A4 and resid 253 and name O)	2.89	0.05	0.05
	assign (segid 3A4 and resid 252 and name N)	(segid 3A4 and resid 254 and name C)	5.75	0.30	0.29
	assign (segid 3A4 and resid 252 and name N)	(segid 3A4 and resid 254 and name CA)	5.52	0.15	0.14
	assign (segid 3A4 and resid 252 and name N)	(segid 3A4 and resid 254 and name N)	4.49	0.14	0.14
60	assign (segid 3A4 and resid 252 and name N)	(segid 3A4 and resid 254 and name O)	6.92	0.30	0.31
	assign (segid 3A4 and resid 252 and name N)	(segid 3A4 and resid 255 and name C)	6.27	0.49	0.50
	assign (segid 3A4 and resid 252 and name N)	(segid 3A4 and resid 255 and name CA)	5.60	0.64	0.65
	assign (segid 3A4 and resid 252 and name N)	(segid 3A4 and resid 255 and name N)	4.90	0.47	0.46
	assign (segid 3A4 and resid 252 and name N)	(segid 3A4 and resid 256 and name CA)	7.01	0.37	0.37
65	assign (segid 3A4 and resid 252 and name N)	(segid 3A4 and resid 256 and name N)	6.03	0.39	0.39
	assign (segid 3A4 and resid 252 and name N)	(segid 3A4 and resid 1 and name C3C)	6.90	0.36	0.35
	assign (segid 3A4 and resid 252 and name N)	(segid 3A4 and resid 1 and name CAC)	6.02	0.42	0.41
	assign (segid 3A4 and resid 252 and name N)	(segid 3A4 and resid 1 and name CBC)	6.02	0.30	0.29
	assign (segid 3A4 and resid 252 and name N)	(segid 3A4 and resid 1 and name CHD)	7.13	0.34	0.35
70	assign (segid 3A4 and resid 252 and name N)	(segid 3A4 and resid 252 and name CB)	3.40	0.04	0.04
	assign (segid 3A4 and resid 252 and name O)	(segid 3A4 and resid 253 and name C)	3.04	0.12	0.11
	assign (segid 3A4 and resid 252 and name O)	(segid 3A4 and resid 253 and name CA)	2.74	0.05	0.05
	assign (segid 3A4 and resid 252 and name O)	(segid 3A4 and resid 253 and name N)	2.25	0.01	0.02
	assign (segid 3A4 and resid 252 and name O)	(segid 3A4 and resid 253 and name O)	3.50	0.18	0.18
75	assign (segid 3A4 and resid 252 and name O)	(segid 3A4 and resid 254 and name C)	4.37	0.30	0.30
	assign (segid 3A4 and resid 252 and name O)	(segid 3A4 and resid 254 and name CA)	4.57	0.15	0.15
	assign (segid 3A4 and resid 252 and name O)	(segid 3A4 and resid 254 and name N)	3.56	0.11	0.12
	assign (segid 3A4 and resid 252 and name O)	(segid 3A4 and resid 254 and name O)	5.31	0.36	0.36
	assign (segid 3A4 and resid 252 and name O)	(segid 3A4 and resid 255 and name C)	3.99	0.40	0.40
80	assign (segid 3A4 and resid 252 and name O)	(segid 3A4 and resid 255 and name CA)	4.08	0.48	0.47
	assign (segid 3A4 and resid 252 and name O)	(segid 3A4 and resid 255 and name N)	3.57	0.35	0.34
	assign (segid 3A4 and resid 252 and name O)	(segid 3A4 and resid 255 and name O)	5.08	0.39	0.39

	assign (segid 3A4 and resid 252 and name O) (segid 3A4 and resid 256 and name C)	5.06	0.36	0.35
	assign (segid 3A4 and resid 252 and name O) (segid 3A4 and resid 256 and name CA)	3.92	0.35	0.35
	assign (segid 3A4 and resid 252 and name O) (segid 3A4 and resid 256 and name N)	3.19	0.38	0.38
	assign (segid 3A4 and resid 252 and name O) (segid 3A4 and resid 256 and name O)	6.15	0.35	0.35
	assign (segid 3A4 and resid 252 and name O) (segid 3A4 and resid 257 and name CA)	6.44	0.41	0.41
5	assign (segid 3A4 and resid 252 and name O) (segid 3A4 and resid 257 and name N)	5.11	0.39	0.38
	assign (segid 3A4 and resid 252 and name O) (segid 3A4 and resid 258 and name N)	7.30	0.35	0.35
	assign (segid 3A4 and resid 252 and name O) (segid HEM and resid 1 and name C2C)	7.30	0.36	0.36
	assign (segid 3A4 and resid 252 and name O) (segid HEM and resid 1 and name C3C)	7.00	0.39	0.39
	assign (segid 3A4 and resid 252 and name O) (segid HEM and resid 1 and name CAC)	6.64	0.45	0.45
	assign (segid 3A4 and resid 252 and name O) (segid HEM and resid 1 and name CBC)	6.82	0.34	0.34
10	assign (segid 3A4 and resid 252 and name O) (segid 3A4 and resid 253 and name O)	1.24	0.01	0.00
	assign (segid 3A4 and resid 253 and name C) (segid 3A4 and resid 254 and name C)	3.07	0.05	0.05
	assign (segid 3A4 and resid 253 and name C) (segid 3A4 and resid 254 and name CA)	2.44	0.01	0.01
	assign (segid 3A4 and resid 253 and name C) (segid 3A4 and resid 254 and name N)	1.33	0.00	0.01
	assign (segid 3A4 and resid 253 and name C) (segid 3A4 and resid 254 and name O)	3.97	0.11	0.10
15	assign (segid 3A4 and resid 253 and name C) (segid 3A4 and resid 255 and name C)	4.79	0.16	0.16
	assign (segid 3A4 and resid 253 and name C) (segid 3A4 and resid 255 and name CA)	4.49	0.11	0.10
	assign (segid 3A4 and resid 253 and name C) (segid 3A4 and resid 255 and name N)	3.28	0.10	0.09
	assign (segid 3A4 and resid 253 and name C) (segid 3A4 and resid 255 and name O)	5.99	0.17	0.16
20	assign (segid 3A4 and resid 253 and name C) (segid 3A4 and resid 256 and name C)	5.60	0.41	0.41
	assign (segid 3A4 and resid 253 and name C) (segid 3A4 and resid 256 and name CA)	5.12	0.24	0.25
	assign (segid 3A4 and resid 253 and name C) (segid 3A4 and resid 256 and name N)	4.14	0.17	0.18
	assign (segid 3A4 and resid 253 and name C) (segid 3A4 and resid 256 and name O)	6.79	0.41	0.42
	assign (segid 3A4 and resid 253 and name C) (segid 3A4 and resid 257 and name C)	6.70	0.67	0.68
25	assign (segid 3A4 and resid 253 and name C) (segid 3A4 and resid 257 and name CA)	5.91	0.67	0.67
	assign (segid 3A4 and resid 253 and name C) (segid 3A4 and resid 257 and name N)	4.98	0.54	0.55
	assign (segid 3A4 and resid 253 and name C) (segid 3A4 and resid 258 and name N)	6.39	0.51	0.50
	assign (segid 3A4 and resid 253 and name C) (segid HEM and resid 1 and name C1C)	7.42	0.21	0.21
	assign (segid 3A4 and resid 253 and name C) (segid HEM and resid 1 and name C2C)	7.27	0.22	0.21
30	assign (segid 3A4 and resid 253 and name C) (segid HEM and resid 1 and name C3C)	6.92	0.23	0.23
	assign (segid 3A4 and resid 253 and name C) (segid HEM and resid 1 and name C4C)	6.90	0.27	0.27
	assign (segid 3A4 and resid 253 and name C) (segid HEM and resid 1 and name CAC)	6.98	0.23	0.24
	assign (segid 3A4 and resid 253 and name C) (segid HEM and resid 1 and name CHD)	6.95	0.29	0.30
	assign (segid 3A4 and resid 253 and name C) (segid HEM and resid 1 and name NC)	7.26	0.26	0.25
35	assign (segid 3A4 and resid 253 and name C) (segid HEM and resid 1 and name NC)	1.53	0.01	0.00
	assign (segid 3A4 and resid 253 and name CA) (segid 3A4 and resid 253 and name O)	2.40	0.01	0.01
	assign (segid 3A4 and resid 253 and name CA) (segid 3A4 and resid 254 and name C)	4.48	0.06	0.05
	assign (segid 3A4 and resid 253 and name CA) (segid 3A4 and resid 254 and name CA)	3.82	0.01	0.02
	assign (segid 3A4 and resid 253 and name CA) (segid 3A4 and resid 254 and name N)	2.45	0.02	0.02
40	assign (segid 3A4 and resid 253 and name CA) (segid 3A4 and resid 254 and name O)	5.43	0.09	0.10
	assign (segid 3A4 and resid 253 and name CA) (segid 3A4 and resid 255 and name C)	5.69	0.16	0.16
	assign (segid 3A4 and resid 253 and name CA) (segid 3A4 and resid 255 and name CA)	5.50	0.16	0.15
	assign (segid 3A4 and resid 253 and name CA) (segid 3A4 and resid 255 and name N)	4.39	0.13	0.13
	assign (segid 3A4 and resid 253 and name CA) (segid 3A4 and resid 255 and name O)	6.88	0.16	0.16
45	assign (segid 3A4 and resid 253 and name CA) (segid 3A4 and resid 256 and name C)	6.26	0.33	0.33
	assign (segid 3A4 and resid 253 and name CA) (segid 3A4 and resid 256 and name CA)	5.65	0.23	0.23
	assign (segid 3A4 and resid 253 and name CA) (segid 3A4 and resid 256 and name N)	4.87	0.16	0.15
	assign (segid 3A4 and resid 253 and name CA) (segid 3A4 and resid 256 and name O)	7.45	0.37	0.36
50	assign (segid 3A4 and resid 253 and name CA) (segid 3A4 and resid 257 and name CA)	6.69	0.58	0.58
	assign (segid 3A4 and resid 253 and name CA) (segid 3A4 and resid 257 and name N)	5.72	0.44	0.44
	assign (segid 3A4 and resid 253 and name CA) (segid 3A4 and resid 258 and name CA)	8.73	0.43	0.43
	assign (segid 3A4 and resid 253 and name CA) (segid 3A4 and resid 258 and name CB)	8.52	0.45	0.45
	assign (segid 3A4 and resid 253 and name CA) (segid 3A4 and resid 259 and name CA)	10.55	0.11	0.11
	assign (segid 3A4 and resid 253 and name CA) (segid 3A4 and resid 259 and name CB)	10.30	0.21	0.22
55	assign (segid 3A4 and resid 253 and name CA) (segid 3A4 and resid 260 and name CA)	11.39	0.30	0.30
	assign (segid 3A4 and resid 253 and name CA) (segid 3A4 and resid 260 and name CB)	10.69	0.41	0.40
	assign (segid 3A4 and resid 253 and name CA) (segid 3A4 and resid 261 and name CA)	12.81	0.40	0.40
	assign (segid 3A4 and resid 253 and name CA) (segid 3A4 and resid 262 and name CA)	14.66	0.27	0.28
	assign (segid 3A4 and resid 253 and name CA) (segid 3A4 and resid 262 and name CB)	14.27	0.23	0.24
60	assign (segid 3A4 and resid 253 and name CA) (segid 3A4 and resid 263 and name CA)	16.28	0.22	0.21
	assign (segid 3A4 and resid 253 and name CA) (segid 3A4 and resid 263 and name CB)	15.76	0.20	0.20
	assign (segid 3A4 and resid 253 and name CA) (segid 3A4 and resid 264 and name CA)	17.36	0.35	0.36
	assign (segid 3A4 and resid 253 and name CA) (segid 3A4 and resid 264 and name CB)	18.74	0.29	0.28
	assign (segid 3A4 and resid 253 and name CA) (segid 3A4 and resid 265 and name CA)	18.61	0.52	0.53
65	assign (segid 3A4 and resid 253 and name CA) (segid 3A4 and resid 313 and name CA)	18.19	0.54	0.54
	assign (segid 3A4 and resid 253 and name CA) (segid 3A4 and resid 317 and name CA)	17.29	0.60	0.61
	assign (segid 3A4 and resid 253 and name CA) (segid 3A4 and resid 318 and name CA)	14.04	0.57	0.56
	assign (segid 3A4 and resid 253 and name CA) (segid 3A4 and resid 318 and name CB)	13.23	0.59	0.59
	assign (segid 3A4 and resid 253 and name CA) (segid 3A4 and resid 319 and name CA)	12.94	0.71	0.72
70	assign (segid 3A4 and resid 253 and name CA) (segid 3A4 and resid 319 and name CB)	12.25	0.68	0.68
	assign (segid 3A4 and resid 253 and name CA) (segid 3A4 and resid 322 and name CA)	17.51	0.68	0.68
	assign (segid 3A4 and resid 253 and name CA) (segid 3A4 and resid 347 and name CB)	18.05	0.98	0.99
	assign (segid 3A4 and resid 253 and name CA) (segid 3A4 and resid 383 and name CA)	17.05	0.33	0.33
	assign (segid 3A4 and resid 253 and name CA) (segid 3A4 and resid 384 and name CA)	15.25	0.36	0.35
75	assign (segid 3A4 and resid 253 and name CA) (segid 3A4 and resid 384 and name CB)	15.57	0.39	0.39
	assign (segid 3A4 and resid 253 and name CA) (segid 3A4 and resid 385 and name CA)	16.72	0.44	0.44
	assign (segid 3A4 and resid 253 and name CA) (segid 3A4 and resid 389 and name CA)	16.16	0.38	0.38
	assign (segid 3A4 and resid 253 and name CA) (segid 3A4 and resid 389 and name CB)	15.90	0.52	0.53
	assign (segid 3A4 and resid 253 and name CA) (segid 3A4 and resid 390 and name CA)	16.10	0.35	0.36
80	assign (segid 3A4 and resid 253 and name CA) (segid 3A4 and resid 390 and name CB)	17.35	0.36	0.36
	assign (segid 3A4 and resid 253 and name CA) (segid 3A4 and resid 391 and name CA)	13.04	0.37	0.36
	assign (segid 3A4 and resid 253 and name CA) (segid 3A4 and resid 391 and name CB)	12.74	0.37	0.37

	assign (segid 3A4 and resid 253 and name CA)	(segid 3A4 and resid 392 and name CA)	13.15	0.35	0.34
	assign (segid 3A4 and resid 253 and name CA)	(segid 3A4 and resid 392 and name CB)	12.61	0.43	0.43
	assign (segid 3A4 and resid 253 and name CA)	(segid 3A4 and resid 393 and name CA)	11.78	0.27	0.26
	assign (segid 3A4 and resid 253 and name CA)	(segid 3A4 and resid 394 and name CA)	14.45	0.26	0.27
	assign (segid 3A4 and resid 253 and name CA)	(segid 3A4 and resid 394 and name CB)	15.48	0.32	0.32
5	assign (segid 3A4 and resid 253 and name CA)	(segid 3A4 and resid 395 and name CA)	16.71	0.22	0.23
	assign (segid 3A4 and resid 253 and name CA)	(segid 3A4 and resid 396 and name CA)	14.46	0.27	0.27
	assign (segid 3A4 and resid 253 and name CA)	(segid 3A4 and resid 396 and name CB)	13.36	0.36	0.37
	assign (segid 3A4 and resid 253 and name CA)	(segid 3A4 and resid 397 and name CA)	13.36	0.16	0.17
	assign (segid 3A4 and resid 253 and name CA)	(segid 3A4 and resid 397 and name CB)	12.81	0.18	0.17
10	assign (segid 3A4 and resid 253 and name CA)	(segid 3A4 and resid 398 and name CA)	17.09	0.18	0.18
	assign (segid 3A4 and resid 253 and name CA)	(segid 3A4 and resid 398 and name CB)	18.02	0.18	0.17
	assign (segid 3A4 and resid 253 and name CA)	(segid 3A4 and resid 399 and name CA)	18.21	0.24	0.25
	assign (segid 3A4 and resid 253 and name CA)	(segid 3A4 and resid 399 and name CB)	18.12	0.30	0.30
	assign (segid 3A4 and resid 253 and name CA)	(segid 3A4 and resid 400 and name CA)	16.18	0.28	0.28
15	assign (segid 3A4 and resid 253 and name CA)	(segid 3A4 and resid 400 and name CB)	14.69	0.29	0.29
	assign (segid 3A4 and resid 253 and name CA)	(segid 3A4 and resid 401 and name CA)	17.37	0.33	0.33
	assign (segid 3A4 and resid 253 and name CA)	(segid 3A4 and resid 401 and name CB)	18.73	0.53	0.52
	assign (segid 3A4 and resid 253 and name CA)	(segid 3A4 and resid 404 and name CA)	12.85	1.80	1.80
	assign (segid 3A4 and resid 253 and name CA)	(segid 3A4 and resid 433 and name CA)	14.61	1.22	1.22
20	assign (segid 3A4 and resid 253 and name CA)	(segid 3A4 and resid 434 and name CA)	15.06	0.59	0.58
	assign (segid 3A4 and resid 253 and name CA)	(segid 3A4 and resid 435 and name CA)	17.50	0.68	0.69
	assign (segid 3A4 and resid 253 and name N)	(segid 3A4 and resid 253 and name C)	2.50	0.03	0.04
	assign (segid 3A4 and resid 253 and name N)	(segid 3A4 and resid 253 and name CA)	1.46	0.01	0.01
	assign (segid 3A4 and resid 253 and name N)	(segid 3A4 and resid 253 and name O)	3.54	0.04	0.04
25	assign (segid 3A4 and resid 253 and name N)	(segid 3A4 and resid 254 and name C)	4.83	0.14	0.14
	assign (segid 3A4 and resid 253 and name N)	(segid 3A4 and resid 254 and name CA)	4.31	0.08	0.07
	assign (segid 3A4 and resid 253 and name N)	(segid 3A4 and resid 254 and name N)	2.89	0.08	0.08
	assign (segid 3A4 and resid 253 and name N)	(segid 3A4 and resid 254 and name O)	5.93	0.12	0.13
	assign (segid 3A4 and resid 253 and name N)	(segid 3A4 and resid 255 and name C)	5.76	0.27	0.27
30	assign (segid 3A4 and resid 253 and name N)	(segid 3A4 and resid 255 and name CA)	5.43	0.34	0.34
	assign (segid 3A4 and resid 253 and name N)	(segid 3A4 and resid 255 and name N)	4.41	0.27	0.26
	assign (segid 3A4 and resid 253 and name N)	(segid 3A4 and resid 255 and name O)	6.95	0.27	0.27
	assign (segid 3A4 and resid 253 and name N)	(segid 3A4 and resid 256 and name C)	6.82	0.32	0.31
	assign (segid 3A4 and resid 253 and name N)	(segid 3A4 and resid 256 and name CA)	5.91	0.26	0.27
35	assign (segid 3A4 and resid 253 and name N)	(segid 3A4 and resid 256 and name N)	5.06	0.24	0.25
	assign (segid 3A4 and resid 253 and name N)	(segid 3A4 and resid 257 and name N)	6.53	0.42	0.41
	assign (segid 3A4 and resid 253 and name N)	(segid 3A4 and resid 257 and name CAC)	7.28	0.33	0.33
	assign (segid 3A4 and resid 253 and name O)	(segid 3A4 and resid 254 and name C)	3.05	0.07	0.08
	assign (segid 3A4 and resid 253 and name O)	(segid 3A4 and resid 254 and name CA)	2.77	0.04	0.03
40	assign (segid 3A4 and resid 253 and name O)	(segid 3A4 and resid 254 and name N)	2.25	0.01	0.02
	assign (segid 3A4 and resid 253 and name O)	(segid 3A4 and resid 254 and name O)	3.61	0.15	0.15
	assign (segid 3A4 and resid 253 and name O)	(segid 3A4 and resid 255 and name C)	4.46	0.15	0.16
	assign (segid 3A4 and resid 253 and name O)	(segid 3A4 and resid 255 and name CA)	4.44	0.13	0.13
	assign (segid 3A4 and resid 253 and name O)	(segid 3A4 and resid 255 and name N)	3.44	0.10	0.11
45	assign (segid 3A4 and resid 253 and name O)	(segid 3A4 and resid 255 and name O)	5.57	0.17	0.16
	assign (segid 3A4 and resid 253 and name O)	(segid 3A4 and resid 256 and name C)	4.73	0.51	0.51
	assign (segid 3A4 and resid 253 and name O)	(segid 3A4 and resid 256 and name CA)	4.54	0.33	0.33
	assign (segid 3A4 and resid 253 and name O)	(segid 3A4 and resid 256 and name N)	3.72	0.22	0.22
	assign (segid 3A4 and resid 253 and name O)	(segid 3A4 and resid 256 and name O)	5.91	0.54	0.53
50	assign (segid 3A4 and resid 253 and name O)	(segid 3A4 and resid 257 and name C)	5.56	0.72	0.73
	assign (segid 3A4 and resid 253 and name O)	(segid 3A4 and resid 257 and name CA)	4.76	0.74	0.75
	assign (segid 3A4 and resid 253 and name O)	(segid 3A4 and resid 257 and name N)	3.95	0.64	0.63
	assign (segid 3A4 and resid 253 and name O)	(segid 3A4 and resid 258 and name CA)	6.45	0.52	0.52
	assign (segid 3A4 and resid 253 and name O)	(segid 3A4 and resid 258 and name CB)	6.27	0.48	0.48
55	assign (segid 3A4 and resid 253 and name O)	(segid 3A4 and resid 258 and name N)	5.32	0.53	0.53
	assign (segid 3A4 and resid 253 and name O)	(segid HEM and resid 1 and name C1C)	7.36	0.20	0.21
	assign (segid 3A4 and resid 253 and name O)	(segid HEM and resid 1 and name C2C)	7.32	0.21	0.22
	assign (segid 3A4 and resid 253 and name O)	(segid HEM and resid 1 and name C3C)	7.19	0.20	0.21
	assign (segid 3A4 and resid 253 and name O)	(segid HEM and resid 1 and name C4C)	7.18	0.24	0.25
60	assign (segid 3A4 and resid 253 and name O)	(segid HEM and resid 1 and name CAC)	7.44	0.21	0.22
	assign (segid 3A4 and resid 253 and name O)	(segid HEM and resid 1 and name CHC)	7.75	0.24	0.23
	assign (segid 3A4 and resid 253 and name O)	(segid HEM and resid 1 and name NC)	7.33	0.24	0.24
	assign (segid 3A4 and resid 254 and name C)	(segid 3A4 and resid 254 and name O)	1.24	0.01	0.01
65	assign (segid 3A4 and resid 254 and name C)	(segid 3A4 and resid 255 and name C)	3.28	0.14	0.15
	assign (segid 3A4 and resid 254 and name C)	(segid 3A4 and resid 255 and name CA)	2.41	0.02	0.01
	assign (segid 3A4 and resid 254 and name C)	(segid 3A4 and resid 255 and name N)	1.32	0.01	0.01
	assign (segid 3A4 and resid 254 and name C)	(segid 3A4 and resid 255 and name O)	4.28	0.18	0.17
	assign (segid 3A4 and resid 254 and name C)	(segid 3A4 and resid 256 and name C)	5.32	0.35	0.35
	assign (segid 3A4 and resid 254 and name C)	(segid 3A4 and resid 256 and name CA)	4.88	0.22	0.22
70	assign (segid 3A4 and resid 254 and name C)	(segid 3A4 and resid 256 and name N)	3.54	0.17	0.17
	assign (segid 3A4 and resid 254 and name C)	(segid 3A4 and resid 256 and name O)	6.31	0.34	0.35
	assign (segid 3A4 and resid 254 and name C)	(segid 3A4 and resid 257 and name C)	6.11	0.51	0.52
	assign (segid 3A4 and resid 254 and name C)	(segid 3A4 and resid 257 and name CA)	5.95	0.52	0.51
	assign (segid 3A4 and resid 254 and name C)	(segid 3A4 and resid 257 and name N)	5.00	0.45	0.46
75	assign (segid 3A4 and resid 254 and name C)	(segid 3A4 and resid 258 and name C)	6.78	0.38	0.38
	assign (segid 3A4 and resid 254 and name C)	(segid 3A4 and resid 258 and name CA)	5.92	0.40	0.39
	assign (segid 3A4 and resid 254 and name C)	(segid 3A4 and resid 258 and name CB)	5.16	0.40	0.39
	assign (segid 3A4 and resid 254 and name C)	(segid 3A4 and resid 258 and name N)	5.28	0.42	0.42
	assign (segid 3A4 and resid 254 and name C)	(segid 3A4 and resid 259 and name N)	6.43	0.39	0.39
80	assign (segid 3A4 and resid 254 and name C)	(segid HEM and resid 1 and name C1B)	6.81	0.35	0.35
	assign (segid 3A4 and resid 254 and name C)	(segid HEM and resid 1 and name C1C)	4.56	0.18	0.19
	assign (segid 3A4 and resid 254 and name C)	(segid HEM and resid 1 and name C1D)	5.38	0.41	0.42

	assign (segid 3A4 and resid 254 and name C) (segid HEM and resid 1 and name C2B)	7.33	0.26	0.27
	assign (segid 3A4 and resid 254 and name C) (segid HEM and resid 1 and name C2C)	4.54	0.28	0.27
	assign (segid 3A4 and resid 254 and name C) (segid HEM and resid 1 and name C2D)	6.30	0.19	0.49
	assign (segid 3A4 and resid 254 and name C) (segid HEM and resid 1 and name C3B)	6.72	0.20	0.20
5	assign (segid 3A4 and resid 254 and name C) (segid HEM and resid 1 and name C3C)	4.37	0.20	0.21
	assign (segid 3A4 and resid 254 and name C) (segid HEM and resid 1 and name C4B)	5.72	0.22	0.22
	assign (segid 3A4 and resid 254 and name C) (segid HEM and resid 1 and name C4C)	4.33	0.18	0.19
	assign (segid 3A4 and resid 254 and name C) (segid HEM and resid 1 and name C4D)	6.64	0.56	0.57
	assign (segid 3A4 and resid 254 and name C) (segid HEM and resid 1 and name CAB)	7.23	0.17	0.18
10	assign (segid 3A4 and resid 254 and name C) (segid HEM and resid 1 and name CAC)	4.84	0.25	0.25
	assign (segid 3A4 and resid 254 and name C) (segid HEM and resid 1 and name CBC)	5.66	0.79	0.78
	assign (segid 3A4 and resid 254 and name C) (segid HEM and resid 1 and name CHC)	5.16	0.17	0.18
	assign (segid 3A4 and resid 254 and name C) (segid HEM and resid 1 and name CHD)	4.73	0.27	0.28
	assign (segid 3A4 and resid 254 and name C) (segid HEM and resid 1 and name CMC)	5.28	0.42	0.42
	assign (segid 3A4 and resid 254 and name C) (segid HEM and resid 1 and name CMD)	6.78	0.43	0.42
15	assign (segid 3A4 and resid 254 and name C) (segid HEM and resid 1 and name FE)	5.49	0.50	0.50
	assign (segid 3A4 and resid 254 and name C) (segid HEM and resid 1 and name NA)	6.80	0.51	0.50
	assign (segid 3A4 and resid 254 and name C) (segid HEM and resid 1 and name NB)	5.83	0.33	0.32
	assign (segid 3A4 and resid 254 and name C) (segid HEM and resid 1 and name NC)	4.50	0.25	0.24
	assign (segid 3A4 and resid 254 and name C) (segid HEM and resid 1 and name ND)	5.65	0.47	0.47
20	assign (segid 3A4 and resid 254 and name CA) (segid 3A4 and resid 254 and name C)	1.52	0.01	0.01
	assign (segid 3A4 and resid 254 and name CA) (segid 3A4 and resid 254 and name O)	2.40	0.02	0.02
	assign (segid 3A4 and resid 254 and name CA) (segid 3A4 and resid 255 and name C)	4.64	0.11	0.11
	assign (segid 3A4 and resid 254 and name CA) (segid 3A4 and resid 255 and name CA)	3.78	0.02	0.02
	assign (segid 3A4 and resid 254 and name CA) (segid 3A4 and resid 255 and name N)	2.42	0.02	0.03
25	assign (segid 3A4 and resid 254 and name CA) (segid 3A4 and resid 255 and name O)	5.71	0.14	0.14
	assign (segid 3A4 and resid 254 and name CA) (segid 3A4 and resid 256 and name C)	6.30	0.40	0.41
	assign (segid 3A4 and resid 254 and name CA) (segid 3A4 and resid 256 and name CA)	5.90	0.20	0.20
	assign (segid 3A4 and resid 254 and name CA) (segid 3A4 and resid 256 and name N)	4.62	0.14	0.14
30	assign (segid 3A4 and resid 254 and name CA) (segid 3A4 and resid 257 and name CA)	6.60	0.71	0.70
	assign (segid 3A4 and resid 254 and name CA) (segid 3A4 and resid 257 and name N)	5.77	0.56	0.57
	assign (segid 3A4 and resid 254 and name CA) (segid 3A4 and resid 258 and name CA)	6.79	0.64	0.64
	assign (segid 3A4 and resid 254 and name CA) (segid 3A4 and resid 258 and name CB)	6.00	0.64	0.63
	assign (segid 3A4 and resid 254 and name CA) (segid 3A4 and resid 258 and name N)	6.12	0.64	0.64
35	assign (segid 3A4 and resid 254 and name CA) (segid 3A4 and resid 259 and name CA)	8.83	0.46	0.47
	assign (segid 3A4 and resid 254 and name CA) (segid 3A4 and resid 259 and name CB)	8.68	0.38	0.39
	assign (segid 3A4 and resid 254 and name CA) (segid 3A4 and resid 260 and name CA)	10.80	0.60	0.61
	assign (segid 3A4 and resid 254 and name CA) (segid 3A4 and resid 260 and name CB)	10.57	0.69	0.69
	assign (segid 3A4 and resid 254 and name CA) (segid 3A4 and resid 261 and name CA)	11.80	0.60	0.59
40	assign (segid 3A4 and resid 254 and name CA) (segid 3A4 and resid 262 and name CA)	12.85	0.50	0.49
	assign (segid 3A4 and resid 254 and name CA) (segid 3A4 and resid 262 and name CB)	12.18	0.46	0.46
	assign (segid 3A4 and resid 254 and name CA) (segid 3A4 and resid 263 and name CA)	14.97	0.53	0.52
	assign (segid 3A4 and resid 254 and name CA) (segid 3A4 and resid 263 and name CB)	14.67	0.53	0.53
	assign (segid 3A4 and resid 254 and name CA) (segid 3A4 and resid 264 and name CA)	16.54	0.59	0.59
45	assign (segid 3A4 and resid 254 and name CA) (segid 3A4 and resid 265 and name CA)	17.32	0.47	0.47
	assign (segid 3A4 and resid 254 and name CA) (segid 3A4 and resid 266 and name CA)	18.76	0.52	0.53
	assign (segid 3A4 and resid 254 and name CA) (segid 3A4 and resid 309 and name CA)	18.72	0.62	0.63
	assign (segid 3A4 and resid 254 and name CA) (segid 3A4 and resid 309 and name CB)	18.19	0.66	0.65
	assign (segid 3A4 and resid 254 and name CA) (segid 3A4 and resid 312 and name CA)	18.58	0.54	0.54
50	assign (segid 3A4 and resid 254 and name CA) (segid 3A4 and resid 312 and name CB)	18.19	0.58	0.58
	assign (segid 3A4 and resid 254 and name CA) (segid 3A4 and resid 313 and name CA)	15.70	0.53	0.53
	assign (segid 3A4 and resid 254 and name CA) (segid 3A4 and resid 313 and name CB)	15.12	0.56	0.57
	assign (segid 3A4 and resid 254 and name CA) (segid 3A4 and resid 314 and name CA)	18.42	0.51	0.51
	assign (segid 3A4 and resid 254 and name CA) (segid 3A4 and resid 316 and name CA)	16.95	0.48	0.49
55	assign (segid 3A4 and resid 254 and name CA) (segid 3A4 and resid 317 and name CA)	14.58	0.52	0.53
	assign (segid 3A4 and resid 254 and name CA) (segid 3A4 and resid 318 and name CA)	11.78	0.59	0.58
	assign (segid 3A4 and resid 254 and name CA) (segid 3A4 and resid 318 and name CB)	11.02	0.69	0.69
	assign (segid 3A4 and resid 254 and name CA) (segid 3A4 and resid 319 and name CA)	10.42	0.64	0.64
	assign (segid 3A4 and resid 254 and name CA) (segid 3A4 and resid 319 and name CB)	9.46	0.64	0.64
60	assign (segid 3A4 and resid 254 and name CA) (segid 3A4 and resid 322 and name CA)	15.42	0.64	0.64
	assign (segid 3A4 and resid 254 and name CA) (segid 3A4 and resid 323 and name CA)	17.77	0.74	0.74
	assign (segid 3A4 and resid 254 and name CA) (segid 3A4 and resid 323 and name CB)	18.30	0.75	0.76
	assign (segid 3A4 and resid 254 and name CA) (segid 3A4 and resid 344 and name CA)	18.60	0.34	0.34
	assign (segid 3A4 and resid 254 and name CA) (segid 3A4 and resid 344 and name CB)	18.75	0.46	0.47
65	assign (segid 3A4 and resid 254 and name CA) (segid 3A4 and resid 345 and name CA)	18.11	0.37	0.36
	assign (segid 3A4 and resid 254 and name CA) (segid 3A4 and resid 345 and name CB)	17.69	0.54	0.55
	assign (segid 3A4 and resid 254 and name CA) (segid 3A4 and resid 346 and name CA)	17.95	0.54	0.55
	assign (segid 3A4 and resid 254 and name CA) (segid 3A4 and resid 347 and name CA)	16.42	0.63	0.63
	assign (segid 3A4 and resid 254 and name CA) (segid 3A4 and resid 347 and name CB)	14.98	0.65	0.64
70	assign (segid 3A4 and resid 254 and name CA) (segid 3A4 and resid 348 and name CA)	17.70	0.70	0.70
	assign (segid 3A4 and resid 254 and name CA) (segid 3A4 and resid 381 and name CA)	19.30	0.33	0.32
	assign (segid 3A4 and resid 254 and name CA) (segid 3A4 and resid 382 and name CA)	16.49	0.20	0.20
	assign (segid 3A4 and resid 254 and name CA) (segid 3A4 and resid 382 and name CB)	17.02	0.20	0.20
	assign (segid 3A4 and resid 254 and name CA) (segid 3A4 and resid 383 and name CA)	13.64	0.27	0.26
75	assign (segid 3A4 and resid 254 and name CA) (segid 3A4 and resid 384 and name CA)	11.60	0.28	0.27
	assign (segid 3A4 and resid 254 and name CA) (segid 3A4 and resid 384 and name CB)	11.90	0.35	0.36
	assign (segid 3A4 and resid 254 and name CA) (segid 3A4 and resid 385 and name CA)	13.15	0.23	0.24
	assign (segid 3A4 and resid 254 and name CA) (segid 3A4 and resid 386 and name CA)	16.14	0.29	0.29
	assign (segid 3A4 and resid 251 and name CA) (segid 3A4 and resid 387 and name CA)	17.47	0.40	0.41
80	assign (segid 3A4 and resid 254 and name CA) (segid 3A4 and resid 388 and name CA)	16.57	0.28	0.27
	assign (segid 3A4 and resid 254 and name CA) (segid 3A4 and resid 388 and name CB)	17.38	0.33	0.34
	assign (segid 3A4 and resid 254 and name CA) (segid 3A4 and resid 389 and name CA)	13.02	0.26	0.27
	assign (segid 3A4 and resid 254 and name CA) (segid 3A4 and resid 389 and name CB)	12.87	0.35	0.36

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assign (segid 3A4 and resid 254 and name CA ) (segid 3A4 and resid 390 and name CA ) 12.56 0.34 0.34
assign (segid 3A4 and resid 254 and name CA ) (segid 3A4 and resid 390 and name CB ) 13.78 0.38 0.37
assign (segid 3A4 and resid 254 and name CA ) (segid 3A4 and resid 391 and name CA ) 9.43 0.35 0.35
assign (segid 3A4 and resid 254 and name CA ) (segid 3A4 and resid 391 and name CB ) 9.08 0.37 0.36
5 assign (segid 3A4 and resid 254 and name CA ) (segid 3A4 and resid 392 and name CA ) 9.96 0.28 0.29
assign (segid 3A4 and resid 254 and name CA ) (segid 3A4 and resid 392 and name CB ) 9.67 0.35 0.34
assign (segid 3A4 and resid 254 and name CA ) (segid 3A4 and resid 393 and name CA ) 8.73 0.51 0.51
assign (segid 3A4 and resid 254 and name CA ) (segid 3A4 and resid 394 and name CA ) 11.09 0.44 0.45
assign (segid 3A4 and resid 254 and name CA ) (segid 3A4 and resid 394 and name CB ) 12.00 0.45 0.45
10 assign (segid 3A4 and resid 254 and name CA ) (segid 3A4 and resid 395 and name CA ) 13.74 0.52 0.52
assign (segid 3A4 and resid 254 and name CA ) (segid 3A4 and resid 396 and name CA ) 12.05 0.65 0.65
assign (segid 3A4 and resid 254 and name CA ) (segid 3A4 and resid 396 and name CB ) 11.12 0.75 0.75
assign (segid 3A4 and resid 254 and name CA ) (segid 3A4 and resid 397 and name CA ) 10.74 0.49 0.49
assign (segid 3A4 and resid 254 and name CA ) (segid 3A4 and resid 397 and name CB ) 9.93 0.44 0.44
assign (segid 3A4 and resid 254 and name CA ) (segid 3A4 and resid 398 and name CA ) 14.33 0.47 0.46
15 assign (segid 3A4 and resid 254 and name CA ) (segid 3A4 and resid 398 and name CB ) 15.08 0.43 0.43
assign (segid 3A4 and resid 254 and name CA ) (segid 3A4 and resid 399 and name CA ) 15.94 0.55 0.55
assign (segid 3A4 and resid 254 and name CA ) (segid 3A4 and resid 399 and name CB ) 15.92 0.54 0.55
assign (segid 3A4 and resid 254 and name CA ) (segid 3A4 and resid 400 and name CA ) 14.46 0.61 0.60
20 assign (segid 3A4 and resid 254 and name CA ) (segid 3A4 and resid 400 and name CB ) 13.07 0.62 0.61
assign (segid 3A4 and resid 254 and name CA ) (segid 3A4 and resid 401 and name CA ) 15.38 0.53 0.53
assign (segid 3A4 and resid 254 and name CA ) (segid 3A4 and resid 404 and name CB ) 17.57 0.62 0.62
assign (segid 3A4 and resid 254 and name CA ) (segid 3A4 and resid 427 and name CA ) 17.96 1.00 0.99
assign (segid 3A4 and resid 254 and name CA ) (segid 3A4 and resid 428 and name CA ) 17.80 0.91 0.91
25 assign (segid 3A4 and resid 254 and name CA ) (segid 3A4 and resid 430 and name CA ) 15.09 1.83 1.83
assign (segid 3A4 and resid 254 and name CA ) (segid 3A4 and resid 431 and name CA ) 11.95 1.59 1.60
assign (segid 3A4 and resid 254 and name CA ) (segid 3A4 and resid 433 and name CA ) 13.49 0.95 0.95
assign (segid 3A4 and resid 254 and name CA ) (segid 3A4 and resid 434 and name CA ) 14.29 0.48 0.49
assign (segid 3A4 and resid 254 and name CA ) (segid 3A4 and resid 435 and name CA ) 17.10 0.62 0.62
30 assign (segid 3A4 and resid 254 and name CA ) (segid HEM and resid 1 and name C1B) 7.33 0.27 0.27
assign (segid 3A4 and resid 254 and name CA ) (segid HEM and resid 1 and name C1C) 5.46 0.37 0.37
assign (segid 3A4 and resid 254 and name CA ) (segid HEM and resid 1 and name C1D) 5.23 0.31 0.32
assign (segid 3A4 and resid 254 and name CA ) (segid HEM and resid 1 and name C2C) 5.54 0.43 0.42
assign (segid 3A4 and resid 254 and name CA ) (segid HEM and resid 1 and name C2D) 5.88 0.41 0.40
35 assign (segid 3A4 and resid 254 and name CA ) (segid HEM and resid 1 and name C3C) 5.12 0.37 0.38
assign (segid 3A4 and resid 254 and name CA ) (segid HEM and resid 1 and name C3D) 6.51 0.44 0.45
assign (segid 3A4 and resid 254 and name CA ) (segid HEM and resid 1 and name C4B) 6.55 0.33 0.34
assign (segid 3A4 and resid 254 and name CA ) (segid HEM and resid 1 and name C4C) 4.80 0.33 0.34
40 assign (segid 3A4 and resid 254 and name CA ) (segid HEM and resid 1 and name C4D) 6.30 0.40 0.41
assign (segid 3A4 and resid 254 and name CA ) (segid HEM and resid 1 and name CAC) 5.48 0.34 0.34
assign (segid 3A4 and resid 254 and name CA ) (segid HEM and resid 1 and name CBC) 6.36 0.87 0.86
assign (segid 3A4 and resid 254 and name CA ) (segid HEM and resid 1 and name CHA) 7.07 0.47 0.46
assign (segid 3A4 and resid 254 and name CA ) (segid HEM and resid 1 and name CHC) 6.15 0.37 0.37
45 assign (segid 3A4 and resid 254 and name CA ) (segid HEM and resid 1 and name CHD) 4.83 0.27 0.28
assign (segid 3A4 and resid 254 and name CA ) (segid HEM and resid 1 and name CMC) 6.48 0.49 0.48
assign (segid 3A4 and resid 254 and name CA ) (segid HEM and resid 1 and name CMD) 6.26 0.41 0.41
assign (segid 3A4 and resid 254 and name CA ) (segid HEM and resid 1 and name FE ) 5.78 0.34 0.33
50 assign (segid 3A4 and resid 254 and name CA ) (segid HEM and resid 1 and name NA ) 6.82 0.30 0.31
assign (segid 3A4 and resid 254 and name CA ) (segid HEM and resid 1 and name NB ) 6.40 0.31 0.30
assign (segid 3A4 and resid 254 and name CA ) (segid HEM and resid 1 and name NC ) 5.08 0.32 0.31
assign (segid 3A4 and resid 254 and name CA ) (segid HEM and resid 1 and name ND ) 5.55 0.34 0.33
55 assign (segid 3A4 and resid 254 and name N ) (segid 3A4 and resid 254 and name C ) 2.46 0.04 0.04
assign (segid 3A4 and resid 254 and name N ) (segid 3A4 and resid 254 and name O ) 1.46 0.01 0.01
assign (segid 3A4 and resid 254 and name N ) (segid 3A4 and resid 254 and name O ) 3.53 0.03 0.03
60 assign (segid 3A4 and resid 254 and name N ) (segid 3A4 and resid 255 and name C ) 4.87 0.15 0.14
assign (segid 3A4 and resid 254 and name N ) (segid 3A4 and resid 255 and name CA ) 4.18 0.10 0.10
assign (segid 3A4 and resid 254 and name N ) (segid 3A4 and resid 255 and name N ) 2.77 0.11 0.10
assign (segid 3A4 and resid 254 and name N ) (segid 3A4 and resid 255 and name O ) 6.06 0.15 0.15
assign (segid 3A4 and resid 254 and name N ) (segid 3A4 and resid 256 and name C ) 6.31 0.34 0.34
65 assign (segid 3A4 and resid 254 and name N ) (segid 3A4 and resid 256 and name CA ) 5.75 0.17 0.16
assign (segid 3A4 and resid 254 and name N ) (segid 3A4 and resid 256 and name N ) 4.55 0.13 0.13
assign (segid 3A4 and resid 254 and name N ) (segid 3A4 and resid 257 and name CA ) 6.73 0.66 0.66
assign (segid 3A4 and resid 254 and name N ) (segid 3A4 and resid 257 and name N ) 5.79 0.52 0.52
70 assign (segid 3A4 and resid 254 and name N ) (segid 3A4 and resid 258 and name N ) 6.77 0.54 0.54
assign (segid 3A4 and resid 254 and name N ) (segid HEM and resid 1 and name C1C) 6.61 0.24 0.24
assign (segid 3A4 and resid 254 and name N ) (segid HEM and resid 1 and name C1D) 6.23 0.34 0.33
assign (segid 3A4 and resid 254 and name N ) (segid HEM and resid 1 and name C2C) 6.47 0.25 0.26
75 assign (segid 3A4 and resid 254 and name N ) (segid HEM and resid 1 and name C2D) 6.69 0.40 0.40
assign (segid 3A4 and resid 254 and name N ) (segid HEM and resid 1 and name C3C) 5.96 0.26 0.27
assign (segid 3A4 and resid 254 and name N ) (segid HEM and resid 1 and name C4C) 5.82 0.29 0.30
80 assign (segid 3A4 and resid 254 and name N ) (segid HEM and resid 1 and name CAC) 6.02 0.24 0.25
assign (segid 3A4 and resid 254 and name N ) (segid HEM and resid 1 and name CBC) 6.74 0.73 0.72
assign (segid 3A4 and resid 254 and name N ) (segid HEM and resid 1 and name CHC) 7.35 0.25 0.25
assign (segid 3A4 and resid 254 and name N ) (segid HEM and resid 1 and name CHD) 5.74 0.30 0.30
assign (segid 3A4 and resid 254 and name N ) (segid HEM and resid 1 and name CMC) 7.27 0.28 0.28
assign (segid 3A4 and resid 254 and name N ) (segid HEM and resid 1 and name CMD) 6.79 0.42 0.42
assign (segid 3A4 and resid 254 and name N ) (segid HEM and resid 1 and name FE ) 7.10 0.33 0.33
assign (segid 3A4 and resid 254 and name N ) (segid HEM and resid 1 and name NC ) 6.28 0.27 0.28
assign (segid 3A4 and resid 254 and name N ) (segid HEM and resid 1 and name ND ) 6.71 0.34 0.34
assign (segid 3A4 and resid 254 and name O ) (segid 3A4 and resid 255 and name C ) 3.38 0.24 0.24
assign (segid 3A4 and resid 254 and name O ) (segid 3A4 and resid 255 and name CA ) 2.74 0.04 0.05
assign (segid 3A4 and resid 254 and name O ) (segid 3A4 and resid 255 and name N ) 2.25 0.02 0.02
assign (segid 3A4 and resid 254 and name O ) (segid 3A4 and resid 255 and name O ) 4.11 0.30 0.30

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	assign (segid 3A4 and resid 254 and name O)	(segid 3A4 and resid 256 and name C)	5.15	0.51	0.50
	assign (segid 3A4 and resid 254 and name O)	(segid 3A4 and resid 256 and name CA)	4.98	0.39	0.39
	assign (segid 3A4 and resid 254 and name O)	(segid 3A4 and resid 256 and name N)	3.80	0.29	0.28
	assign (segid 3A4 and resid 254 and name O)	(segid 3A4 and resid 256 and name O)	6.01	0.53	0.53
5	assign (segid 3A4 and resid 254 and name O)	(segid 3A4 and resid 257 and name C)	5.47	0.64	0.64
	assign (segid 3A4 and resid 254 and name O)	(segid 3A4 and resid 257 and name CA)	5.56	0.60	0.60
	assign (segid 3A4 and resid 254 and name O)	(segid 3A4 and resid 257 and name N)	4.80	0.56	0.56
	assign (segid 3A4 and resid 254 and name O)	(segid 3A4 and resid 257 and name O)	6.51	0.73	0.73
	assign (segid 3A4 and resid 254 and name O)	(segid 3A4 and resid 258 and name C)	5.83	0.61	0.60
10	assign (segid 3A4 and resid 254 and name O)	(segid 3A4 and resid 258 and name CA)	4.95	0.55	0.56
	assign (segid 3A4 and resid 254 and name O)	(segid 3A4 and resid 258 and name CB)	4.12	0.52	0.52
	assign (segid 3A4 and resid 254 and name O)	(segid 3A4 and resid 258 and name N)	4.49	0.58	0.58
	assign (segid 3A4 and resid 254 and name O)	(segid 3A4 and resid 259 and name N)	5.57	0.67	0.67
	assign (segid 3A4 and resid 254 and name O)	(segid HEM and resid 1 and name C1B)	5.95	0.49	0.49
15	assign (segid 3A4 and resid 254 and name O)	(segid HEM and resid 1 and name C1C)	4.15	0.46	0.45
	assign (segid 3A4 and resid 254 and name O)	(segid HEM and resid 1 and name C1D)	5.59	0.44	0.43
	assign (segid 3A4 and resid 254 and name O)	(segid HEM and resid 1 and name C2B)	6.36	0.40	0.41
	assign (segid 3A4 and resid 254 and name O)	(segid HEM and resid 1 and name C2C)	4.37	0.56	0.56
	assign (segid 3A4 and resid 254 and name O)	(segid HEM and resid 1 and name C2D)	6.64	0.50	0.51
20	assign (segid 3A4 and resid 254 and name O)	(segid HEM and resid 1 and name C3B)	5.77	0.39	0.40
	assign (segid 3A4 and resid 254 and name O)	(segid HEM and resid 1 and name C3C)	4.53	0.44	0.43
	assign (segid 3A4 and resid 254 and name O)	(segid HEM and resid 1 and name C4B)	4.89	0.42	0.43
	assign (segid 3A4 and resid 254 and name O)	(segid HEM and resid 1 and name C4C)	4.42	0.32	0.32
	assign (segid 3A4 and resid 254 and name O)	(segid HEM and resid 1 and name C4B)	6.27	0.41	0.41
25	assign (segid 3A4 and resid 254 and name O)	(segid HEM and resid 1 and name C4C)	5.27	0.46	0.45
	assign (segid 3A4 and resid 254 and name O)	(segid HEM and resid 1 and name CBC)	6.14	0.86	0.86
	assign (segid 3A4 and resid 254 and name O)	(segid HEM and resid 1 and name CHB)	6.73	0.55	0.55
	assign (segid 3A4 and resid 254 and name O)	(segid HEM and resid 1 and name CHC)	4.47	0.46	0.46
	assign (segid 3A4 and resid 254 and name O)	(segid HEM and resid 1 and name CHD)	5.03	0.31	0.31
30	assign (segid 3A4 and resid 254 and name O)	(segid HEM and resid 1 and name CMC)	5.06	0.73	0.74
	assign (segid 3A4 and resid 254 and name O)	(segid HEM and resid 1 and name FE)	5.05	0.59	0.59
	assign (segid 3A4 and resid 254 and name O)	(segid HEM and resid 1 and name NA)	6.29	0.64	0.63
	assign (segid 3A4 and resid 254 and name O)	(segid HEM and resid 1 and name NB)	5.06	0.47	0.47
	assign (segid 3A4 and resid 254 and name O)	(segid HEM and resid 1 and name NC)	4.23	0.40	0.40
35	assign (segid 3A4 and resid 254 and name O)	(segid HEM and resid 1 and name ND)	5.59	0.53	0.54
	assign (segid 3A4 and resid 255 and name C)	(segid 3A4 and resid 255 and name O)	1.24	0.01	0.01
	assign (segid 3A4 and resid 255 and name C)	(segid 3A4 and resid 256 and name C)	3.26	0.14	0.13
	assign (segid 3A4 and resid 255 and name C)	(segid 3A4 and resid 256 and name CA)	2.40	0.02	0.02
	assign (segid 3A4 and resid 255 and name C)	(segid 3A4 and resid 256 and name N)	1.33	0.01	0.01
40	assign (segid 3A4 and resid 255 and name C)	(segid 3A4 and resid 256 and name O)	4.01	0.23	0.24
	assign (segid 3A4 and resid 255 and name C)	(segid 3A4 and resid 257 and name C)	5.30	0.32	0.31
	assign (segid 3A4 and resid 255 and name C)	(segid 3A4 and resid 257 and name CA)	5.04	0.20	0.20
	assign (segid 3A4 and resid 255 and name C)	(segid 3A4 and resid 257 and name N)	3.77	0.17	0.18
	assign (segid 3A4 and resid 255 and name C)	(segid 3A4 and resid 257 and name O)	6.29	0.33	0.34
45	assign (segid 3A4 and resid 255 and name C)	(segid 3A4 and resid 258 and name C)	5.82	0.52	0.52
	assign (segid 3A4 and resid 255 and name C)	(segid 3A4 and resid 258 and name CA)	5.57	0.54	0.53
	assign (segid 3A4 and resid 255 and name C)	(segid 3A4 and resid 258 and name CB)	5.41	0.65	0.64
	assign (segid 3A4 and resid 255 and name C)	(segid 3A4 and resid 258 and name N)	4.78	0.44	0.43
	assign (segid 3A4 and resid 255 and name C)	(segid 3A4 and resid 258 and name O)	6.99	0.50	0.49
50	assign (segid 3A4 and resid 255 and name C)	(segid 3A4 and resid 259 and name C)	6.64	0.38	0.37
	assign (segid 3A4 and resid 255 and name C)	(segid 3A4 and resid 259 and name CA)	5.75	0.50	0.50
	assign (segid 3A4 and resid 255 and name C)	(segid 3A4 and resid 259 and name CB)	5.17	0.55	0.56
	assign (segid 3A4 and resid 255 and name C)	(segid 3A4 and resid 259 and name N)	5.00	0.53	0.52
	assign (segid 3A4 and resid 255 and name C)	(segid 3A4 and resid 260 and name N)	6.36	0.29	0.29
55	assign (segid 3A4 and resid 255 and name C)	(segid HEM and resid 1 and name C1C)	5.23	0.64	0.65
	assign (segid 3A4 and resid 255 and name C)	(segid HEM and resid 1 and name C2C)	4.70	0.51	0.51
	assign (segid 3A4 and resid 255 and name C)	(segid HEM and resid 1 and name C3C)	5.10	0.45	0.46
	assign (segid 3A4 and resid 255 and name C)	(segid HEM and resid 1 and name C4C)	5.82	0.53	0.54
	assign (segid 3A4 and resid 255 and name C)	(segid HEM and resid 1 and name C4C)	5.35	0.39	0.39
60	assign (segid 3A4 and resid 255 and name C)	(segid HEM and resid 1 and name CBC)	5.65	0.41	0.41
	assign (segid 3A4 and resid 255 and name C)	(segid HEM and resid 1 and name CHC)	5.49	0.72	0.72
	assign (segid 3A4 and resid 255 and name C)	(segid HEM and resid 1 and name CHD)	6.70	0.54	0.53
	assign (segid 3A4 and resid 255 and name C)	(segid HEM and resid 1 and name CMC)	4.47	0.41	0.42
	assign (segid 3A4 and resid 255 and name C)	(segid HEM and resid 1 and name NC)	5.93	0.66	0.66
65	assign (segid 3A4 and resid 255 and name CA)	(segid 3A4 and resid 255 and name C)	1.51	0.00	0.00
	assign (segid 3A4 and resid 255 and name CA)	(segid 3A4 and resid 255 and name O)	2.36	0.02	0.03
	assign (segid 3A4 and resid 255 and name CA)	(segid 3A4 and resid 256 and name C)	4.63	0.10	0.09
	assign (segid 3A4 and resid 255 and name CA)	(segid 3A4 and resid 256 and name CA)	3.79	0.02	0.02
	assign (segid 3A4 and resid 255 and name CA)	(segid 3A4 and resid 256 and name N)	2.46	0.03	0.03
70	assign (segid 3A4 and resid 255 and name CA)	(segid 3A4 and resid 256 and name O)	5.45	0.23	0.22
	assign (segid 3A4 and resid 255 and name CA)	(segid 3A4 and resid 257 and name C)	6.26	0.28	0.29
	assign (segid 3A4 and resid 255 and name CA)	(segid 3A4 and resid 257 and name CA)	6.09	0.17	0.17
	assign (segid 3A4 and resid 255 and name CA)	(segid 3A4 and resid 257 and name N)	4.89	0.15	0.15
	assign (segid 3A4 and resid 255 and name CA)	(segid 3A4 and resid 257 and name O)	7.30	0.31	0.30
75	assign (segid 3A4 and resid 255 and name CA)	(segid 3A4 and resid 258 and name C)	6.57	0.51	0.52
	assign (segid 3A4 and resid 255 and name CA)	(segid 3A4 and resid 258 and name CA)	6.16	0.53	0.54
	assign (segid 3A4 and resid 255 and name CA)	(segid 3A4 and resid 258 and name CB)	5.63	0.69	0.69
	assign (segid 3A4 and resid 255 and name CA)	(segid 3A4 and resid 258 and name N)	5.54	0.41	0.41
	assign (segid 3A4 and resid 255 and name CA)	(segid 3A4 and resid 259 and name CA)	6.67	0.46	0.45
80	assign (segid 3A4 and resid 255 and name CA)	(segid 3A4 and resid 259 and name CB)	6.08	0.45	0.46
	assign (segid 3A4 and resid 255 and name CA)	(segid 3A4 and resid 259 and name N)	5.85	0.48	0.48
	assign (segid 3A4 and resid 255 and name CA)	(segid 3A4 and resid 260 and name CA)	8.83	0.29	0.28
	assign (segid 3A4 and resid 255 and name CA)	(segid 3A4 and resid 260 and name CB)	8.76	0.39	0.40

assign (segid 3A4 and resid 255 and name CA) (segid 3A4 and resid 261 and name CA) 10.70 0.43 0.43
 assign (segid 3A4 and resid 255 and name CA) (segid 3A4 and resid 262 and name CA) 11.35 0.53 0.54
 assign (segid 3A4 and resid 255 and name CA) (segid 3A4 and resid 262 and name CB) 10.59 0.58 0.58
 assign (segid 3A4 and resid 255 and name CA) (segid 3A4 and resid 263 and name CA) 12.81 0.32 0.31
 assign (segid 3A4 and resid 255 and name CA) (segid 3A4 and resid 263 and name CB) 12.29 0.25 0.25
 5 assign (segid 3A4 and resid 255 and name CA) (segid 3A4 and resid 264 and name CA) 14.84 0.35 0.35
 assign (segid 3A4 and resid 255 and name CA) (segid 3A4 and resid 265 and name CA) 16.06 0.62 0.61
 assign (segid 3A4 and resid 255 and name CA) (segid 3A4 and resid 266 and name CA) 17.00 0.44 0.45
 assign (segid 3A4 and resid 255 and name CA) (segid 3A4 and resid 267 and name CA) 19.01 0.22 0.22
 assign (segid 3A4 and resid 255 and name CA) (segid 3A4 and resid 267 and name CB) 18.60 0.23 0.23
 10 assign (segid 3A4 and resid 255 and name CA) (segid 3A4 and resid 309 and name CA) 16.84 0.96 0.96
 assign (segid 3A4 and resid 255 and name CA) (segid 3A4 and resid 309 and name CB) 16.14 0.97 0.97
 assign (segid 3A4 and resid 255 and name CA) (segid 3A4 and resid 310 and name CA) 17.67 0.93 0.93
 assign (segid 3A4 and resid 255 and name CA) (segid 3A4 and resid 312 and name CA) 17.36 1.06 1.06
 assign (segid 3A4 and resid 255 and name CA) (segid 3A4 and resid 312 and name CB) 16.73 1.06 1.07
 15 assign (segid 3A4 and resid 255 and name CA) (segid 3A4 and resid 313 and name CA) 14.88 1.06 1.07
 assign (segid 3A4 and resid 255 and name CA) (segid 3A4 and resid 313 and name CB) 14.24 1.07 1.07
 assign (segid 3A4 and resid 255 and name CA) (segid 3A4 and resid 316 and name CA) 16.70 1.17 1.17
 assign (segid 3A4 and resid 255 and name CA) (segid 3A4 and resid 317 and name CA) 14.83 1.23 1.24
 assign (segid 3A4 and resid 255 and name CA) (segid 3A4 and resid 318 and name CA) 12.16 1.34 1.35
 20 assign (segid 3A4 and resid 255 and name CA) (segid 3A4 and resid 318 and name CB) 11.08 1.27 1.26
 assign (segid 3A4 and resid 255 and name CA) (segid 3A4 and resid 319 and name CA) 11.79 1.55 1.56
 assign (segid 3A4 and resid 255 and name CA) (segid 3A4 and resid 319 and name CB) 10.90 1.62 1.62
 assign (segid 3A4 and resid 255 and name CA) (segid 3A4 and resid 347 and name CA) 17.79 0.89 0.89
 assign (segid 3A4 and resid 255 and name CA) (segid 3A4 and resid 347 and name CB) 16.32 0.85 0.84
 25 assign (segid 3A4 and resid 255 and name CA) (segid 3A4 and resid 382 and name CA) 17.09 0.97 0.96
 assign (segid 3A4 and resid 255 and name CA) (segid 3A4 and resid 382 and name CB) 17.88 0.96 0.97
 assign (segid 3A4 and resid 255 and name CA) (segid 3A4 and resid 383 and name CA) 13.95 0.97 0.97
 assign (segid 3A4 and resid 255 and name CA) (segid 3A4 and resid 384 and name CA) 11.97 0.93 0.93
 assign (segid 3A4 and resid 255 and name CA) (segid 3A4 and resid 384 and name CB) 11.95 0.93 0.93
 30 assign (segid 3A4 and resid 255 and name CA) (segid 3A4 and resid 385 and name CA) 14.37 0.90 0.89
 assign (segid 3A4 and resid 255 and name CA) (segid 3A4 and resid 386 and name CA) 17.35 0.93 0.93
 assign (segid 3A4 and resid 255 and name CA) (segid 3A4 and resid 388 and name CA) 18.13 0.74 0.73
 assign (segid 3A4 and resid 255 and name CA) (segid 3A4 and resid 389 and name CA) 14.88 0.64 0.65
 assign (segid 3A4 and resid 255 and name CA) (segid 3A4 and resid 389 and name CB) 15.03 0.64 0.63
 35 assign (segid 3A4 and resid 255 and name CA) (segid 3A4 and resid 390 and name CA) 13.67 0.80 0.81
 assign (segid 3A4 and resid 255 and name CA) (segid 3A4 and resid 390 and name CB) 14.62 0.87 0.87
 assign (segid 3A4 and resid 255 and name CA) (segid 3A4 and resid 391 and name CA) 10.07 0.79 0.79
 assign (segid 3A4 and resid 255 and name CA) (segid 3A4 and resid 391 and name CB) 9.42 0.86 0.86
 assign (segid 3A4 and resid 255 and name CA) (segid 3A4 and resid 392 and name CA) 10.06 0.59 0.59
 40 assign (segid 3A4 and resid 255 and name CA) (segid 3A4 and resid 392 and name CB) 9.99 0.63 0.63
 assign (segid 3A4 and resid 255 and name CA) (segid 3A4 and resid 393 and name CA) 7.62 0.48 0.48
 assign (segid 3A4 and resid 255 and name CA) (segid 3A4 and resid 394 and name CA) 9.91 0.48 0.49
 assign (segid 3A4 and resid 255 and name CA) (segid 3A4 and resid 394 and name CB) 11.12 0.50 0.51
 45 assign (segid 3A4 and resid 255 and name CA) (segid 3A4 and resid 395 and name CA) 11.85 0.44 0.44
 assign (segid 3A4 and resid 255 and name CA) (segid 3A4 and resid 396 and name CA) 9.52 0.55 0.56
 assign (segid 3A4 and resid 255 and name CA) (segid 3A4 and resid 396 and name CB) 8.59 0.66 0.67
 assign (segid 3A4 and resid 255 and name CA) (segid 3A4 and resid 397 and name CA) 8.29 0.50 0.49
 assign (segid 3A4 and resid 255 and name CA) (segid 3A4 and resid 397 and name CB) 7.84 0.61 0.60
 50 assign (segid 3A4 and resid 255 and name CA) (segid 3A4 and resid 398 and name CA) 12.00 0.50 0.50
 assign (segid 3A4 and resid 255 and name CA) (segid 3A4 and resid 398 and name CB) 12.94 0.53 0.53
 assign (segid 3A4 and resid 255 and name CA) (segid 3A4 and resid 399 and name CA) 13.11 0.46 0.45
 assign (segid 3A4 and resid 255 and name CA) (segid 3A4 and resid 399 and name CB) 13.06 0.53 0.53
 assign (segid 3A4 and resid 255 and name CA) (segid 3A4 and resid 400 and name CA) 11.34 0.46 0.46
 55 assign (segid 3A4 and resid 255 and name CA) (segid 3A4 and resid 400 and name CB) 9.92 0.47 0.48
 assign (segid 3A4 and resid 255 and name CA) (segid 3A4 and resid 401 and name CA) 12.62 0.55 0.55
 assign (segid 3A4 and resid 255 and name CA) (segid 3A4 and resid 402 and name CA) 15.96 0.50 0.50
 assign (segid 3A4 and resid 255 and name CA) (segid 3A4 and resid 402 and name CB) 16.36 0.49 0.50
 assign (segid 3A4 and resid 255 and name CA) (segid 3A4 and resid 403 and name CA) 16.43 0.42 0.42
 60 assign (segid 3A4 and resid 255 and name CA) (segid 3A4 and resid 403 and name CB) 15.79 0.42 0.42
 assign (segid 3A4 and resid 255 and name CA) (segid 3A4 and resid 404 and name CA) 15.73 0.50 0.51
 assign (segid 3A4 and resid 255 and name CA) (segid 3A4 and resid 404 and name CB) 14.51 0.53 0.53
 assign (segid 3A4 and resid 255 and name CA) (segid 3A4 and resid 405 and name CA) 17.91 0.69 0.70
 assign (segid 3A4 and resid 255 and name CA) (segid 3A4 and resid 405 and name CB) 17.73 0.74 0.73
 65 assign (segid 3A4 and resid 255 and name CA) (segid 3A4 and resid 429 and name CA) 17.71 1.04 1.03
 assign (segid 3A4 and resid 255 and name CA) (segid 3A4 and resid 430 and name CA) 17.02 1.36 1.37
 assign (segid 3A4 and resid 255 and name CA) (segid 3A4 and resid 431 and name CA) 14.13 1.01 1.02
 assign (segid 3A4 and resid 255 and name CA) (segid 3A4 and resid 433 and name CA) 14.19 0.84 0.84
 assign (segid 3A4 and resid 255 and name CA) (segid 3A4 and resid 434 and name CA) 14.25 0.74 0.73
 70 assign (segid 3A4 and resid 255 and name CA) (segid 3A4 and resid 435 and name CA) 16.59 0.83 0.82
 assign (segid 3A4 and resid 255 and name CA) (segid HEM and resid 1 and name C1C) 4.41 0.70 0.70
 assign (segid 3A4 and resid 255 and name CA) (segid HEM and resid 1 and name C1D) 6.39 0.68 0.68
 assign (segid 3A4 and resid 255 and name CA) (segid HEM and resid 1 and name C2C) 3.86 0.49 0.49
 assign (segid 3A4 and resid 255 and name CA) (segid HEM and resid 1 and name C3C) 3.97 0.47 0.47
 assign (segid 3A4 and resid 255 and name CA) (segid HEM and resid 1 and name C4B) 5.91 0.90 0.90
 75 assign (segid 3A4 and resid 255 and name CA) (segid HEM and resid 1 and name C4C) 4.59 0.60 0.60
 assign (segid 3A4 and resid 255 and name CA) (segid HEM and resid 1 and name CAC) 4.18 0.42 0.43
 assign (segid 3A4 and resid 255 and name CA) (segid HEM and resid 1 and name CBC) 4.64 0.61 0.60
 assign (segid 3A4 and resid 255 and name CA) (segid HEM and resid 1 and name CHC) 4.97 0.76 0.77
 assign (segid 3A4 and resid 255 and name CA) (segid HEM and resid 1 and name CHD) 5.35 0.60 0.60
 80 assign (segid 3A4 and resid 255 and name CA) (segid HEM and resid 1 and name CMC) 4.04 0.34 0.33
 assign (segid 3A4 and resid 255 and name CA) (segid HEM and resid 1 and name NC) 4.87 0.77 0.76
 assign (segid 3A4 and resid 255 and name N) (segid 3A4 and resid 255 and name C) 2.52 0.02 0.02

5	assign (segid 3A4 and resid 255 and name N) (segid 3A4 and resid 255 and name C)	1.45	0.01	0.01
	assign (segid 3A4 and resid 255 and name N) (segid 3A4 and resid 256 and name O)	3.61	0.02	0.02
	assign (segid 3A4 and resid 255 and name N) (segid 3A4 and resid 256 and name C)	5.08	0.07	0.08
	assign (segid 3A4 and resid 255 and name N) (segid 3A4 and resid 256 and name N)	4.32	0.04	0.03
	assign (segid 3A4 and resid 255 and name N) (segid 3A4 and resid 256 and name O)	2.88	0.03	0.04
	assign (segid 3A4 and resid 255 and name N) (segid 3A4 and resid 257 and name C)	6.08	0.13	0.12
	assign (segid 3A4 and resid 255 and name N) (segid 3A4 and resid 257 and name N)	6.49	0.19	0.19
	assign (segid 3A4 and resid 255 and name N) (segid 3A4 and resid 257 and name O)	6.19	0.22	0.22
10	assign (segid 3A4 and resid 255 and name N) (segid 3A4 and resid 258 and name C)	5.04	0.20	0.19
	assign (segid 3A4 and resid 255 and name N) (segid 3A4 and resid 258 and name N)	7.57	0.31	0.31
	assign (segid 3A4 and resid 255 and name N) (segid 3A4 and resid 258 and name O)	7.15	0.19	0.19
	assign (segid 3A4 and resid 255 and name N) (segid 3A4 and resid 258 and name CB)	6.48	0.20	0.21
	assign (segid 3A4 and resid 255 and name N) (segid 3A4 and resid 258 and name N)	5.85	0.33	0.34
	assign (segid 3A4 and resid 255 and name N) (segid 3A4 and resid 259 and name C)	5.77	0.12	0.12
15	assign (segid 3A4 and resid 255 and name N) (segid 3A4 and resid 259 and name N)	7.58	0.20	0.19
	assign (segid 3A4 and resid 255 and name N) (segid 3A4 and resid 259 and name CB)	7.13	0.24	0.24
	assign (segid 3A4 and resid 255 and name N) (segid 3A4 and resid 259 and name N)	6.60	0.19	0.18
	assign (segid 3A4 and resid 255 and name N) (segid HEM and resid 1 and name C1C)	4.70	0.37	0.37
	assign (segid 3A4 and resid 255 and name N) (segid HEM and resid 1 and name C1D)	5.76	0.55	0.56
20	assign (segid 3A4 and resid 255 and name N) (segid HEM and resid 1 and name C2C)	4.32	0.19	0.18
	assign (segid 3A4 and resid 255 and name N) (segid HEM and resid 1 and name C2D)	6.68	0.57	0.57
	assign (segid 3A4 and resid 255 and name N) (segid HEM and resid 1 and name C3C)	4.10	0.21	0.21
	assign (segid 3A4 and resid 255 and name N) (segid HEM and resid 1 and name C4B)	6.21	0.48	0.49
	assign (segid 3A4 and resid 255 and name N) (segid HEM and resid 1 and name C4C)	4.40	0.39	0.39
25	assign (segid 3A4 and resid 255 and name N) (segid HEM and resid 1 and name CAC)	4.28	0.13	0.12
	assign (segid 3A4 and resid 255 and name N) (segid HEM and resid 1 and name CBC)	4.90	0.62	0.63
	assign (segid 3A4 and resid 255 and name N) (segid HEM and resid 1 and name CHC)	5.42	0.39	0.38
	assign (segid 3A4 and resid 255 and name N) (segid HEM and resid 1 and name CHD)	4.87	0.46	0.46
	assign (segid 3A4 and resid 255 and name N) (segid HEM and resid 1 and name CNC)	4.86	0.08	0.07
30	assign (segid 3A4 and resid 255 and name N) (segid HEM and resid 1 and name CHD)	6.95	0.49	0.50
	assign (segid 3A4 and resid 255 and name N) (segid HEM and resid 1 and name FE)	6.14	0.69	0.68
	assign (segid 3A4 and resid 255 and name N) (segid HEM and resid 1 and name NB)	6.48	0.57	0.58
	assign (segid 3A4 and resid 255 and name N) (segid HEM and resid 1 and name NC)	4.80	0.49	0.49
	assign (segid 3A4 and resid 255 and name N) (segid HEM and resid 1 and name ND)	6.24	0.61	0.61
35	assign (segid 3A4 and resid 255 and name O) (segid 3A4 and resid 256 and name C)	3.35	0.26	0.25
	assign (segid 3A4 and resid 255 and name O) (segid 3A4 and resid 256 and name CA)	2.71	0.04	0.05
	assign (segid 3A4 and resid 255 and name O) (segid 3A4 and resid 256 and name N)	2.25	0.01	0.01
	assign (segid 3A4 and resid 255 and name O) (segid 3A4 and resid 256 and name O)	3.75	0.38	0.37
40	assign (segid 3A4 and resid 255 and name O) (segid 3A4 and resid 257 and name C)	5.26	0.56	0.55
	assign (segid 3A4 and resid 255 and name O) (segid 3A4 and resid 257 and name CA)	5.23	0.39	0.38
	assign (segid 3A4 and resid 255 and name O) (segid 3A4 and resid 257 and name N)	4.10	0.31	0.32
	assign (segid 3A4 and resid 255 and name O) (segid 3A4 and resid 257 and name O)	6.14	0.61	0.61
	assign (segid 3A4 and resid 255 and name O) (segid 3A4 and resid 258 and name C)	5.29	0.78	0.78
	assign (segid 3A4 and resid 255 and name O) (segid 3A4 and resid 258 and name CA)	5.34	0.80	0.81
45	assign (segid 3A4 and resid 255 and name O) (segid 3A4 and resid 258 and name CB)	5.30	0.90	0.89
	assign (segid 3A4 and resid 255 and name O) (segid 3A4 and resid 258 and name N)	4.74	0.68	0.68
	assign (segid 3A4 and resid 255 and name O) (segid 3A4 and resid 258 and name O)	6.40	0.75	0.74
	assign (segid 3A4 and resid 255 and name O) (segid 3A4 and resid 259 and name C)	5.75	0.53	0.54
	assign (segid 3A4 and resid 255 and name O) (segid 3A4 and resid 259 and name CA)	4.86	0.67	0.67
50	assign (segid 3A4 and resid 255 and name O) (segid 3A4 and resid 259 and name CB)	4.18	0.66	0.66
	assign (segid 3A4 and resid 255 and name O) (segid 3A4 and resid 259 and name N)	4.31	0.75	0.76
	assign (segid 3A4 and resid 255 and name O) (segid 3A4 and resid 259 and name O)	6.86	0.52	0.53
	assign (segid 3A4 and resid 255 and name O) (segid 3A4 and resid 260 and name CA)	6.78	0.46	0.46
	assign (segid 3A4 and resid 255 and name O) (segid			

	assign (segid 3A4 and resid 256 and name C) (segid 3A4 and resid 261 and name CA)	7.39	0.23	0.23
	assign (segid 3A4 and resid 256 and name C) (segid 3A4 and resid 261 and name N)	6.15	0.23	0.23
	assign (segid 3A4 and resid 256 and name C) (segid HEM and resid 1 and name CMC)	7.01	0.42	0.41
	assign (segid 3A4 and resid 256 and name CA) (segid 3A4 and resid 256 and name C)	1.51	0.01	0.02
	assign (segid 3A4 and resid 256 and name CA) (segid 3A4 and resid 256 and name O)	2.37	0.02	0.03
5	assign (segid 3A4 and resid 256 and name CA) (segid 3A4 and resid 257 and name C)	4.55	0.10	0.10
	assign (segid 3A4 and resid 256 and name CA) (segid 3A4 and resid 257 and name CA)	3.81	0.03	0.02
	assign (segid 3A4 and resid 256 and name CA) (segid 3A4 and resid 257 and name N)	2.44	0.01	0.01
	assign (segid 3A4 and resid 256 and name CA) (segid 3A4 and resid 257 and name O)	5.45	0.20	0.20
	assign (segid 3A4 and resid 256 and name CA) (segid 3A4 and resid 258 and name C)	5.96	0.38	0.38
10	assign (segid 3A4 and resid 256 and name CA) (segid 3A4 and resid 258 and name CA)	5.79	0.26	0.25
	assign (segid 3A4 and resid 256 and name CA) (segid 3A4 and resid 258 and name CB)	6.21	0.31	0.30
	assign (segid 3A4 and resid 256 and name CA) (segid 3A4 and resid 258 and name N)	4.64	0.20	0.20
	assign (segid 3A4 and resid 256 and name CA) (segid 3A4 and resid 258 and name O)	7.02	0.29	0.29
	assign (segid 3A4 and resid 256 and name CA) (segid 3A4 and resid 259 and name C)	6.26	0.51	0.50
15	assign (segid 3A4 and resid 256 and name CA) (segid 3A4 and resid 259 and name CA)	5.87	0.65	0.66
	assign (segid 3A4 and resid 256 and name CA) (segid 3A4 and resid 259 and name CB)	5.45	0.86	0.86
	assign (segid 3A4 and resid 256 and name CA) (segid 3A4 and resid 259 and name N)	5.20	0.56	0.56
	assign (segid 3A4 and resid 256 and name CA) (segid 3A4 and resid 260 and name CA)	6.39	0.18	0.19
	assign (segid 3A4 and resid 256 and name CA) (segid 3A4 and resid 260 and name CB)	5.88	0.14	0.13
20	assign (segid 3A4 and resid 256 and name CA) (segid 3A4 and resid 260 and name N)	5.57	0.36	0.36
	assign (segid 3A4 and resid 256 and name CA) (segid 3A4 and resid 261 and name CA)	8.80	0.21	0.21
	assign (segid 3A4 and resid 256 and name CA) (segid 3A4 and resid 262 and name CA)	10.36	0.44	0.44
	assign (segid 3A4 and resid 256 and name CA) (segid 3A4 and resid 262 and name CB)	10.03	0.55	0.55
	assign (segid 3A4 and resid 256 and name CA) (segid 3A4 and resid 263 and name CA)	11.21	0.46	0.45
25	assign (segid 3A4 and resid 256 and name CA) (segid 3A4 and resid 263 and name CB)	10.50	0.46	0.47
	assign (segid 3A4 and resid 256 and name CA) (segid 3A4 and resid 264 and name CA)	12.65	0.40	0.41
	assign (segid 3A4 and resid 256 and name CA) (segid 3A4 and resid 265 and name CA)	14.52	0.49	0.49
	assign (segid 3A4 and resid 256 and name CA) (segid 3A4 and resid 266 and name CA)	15.80	0.54	0.54
	assign (segid 3A4 and resid 256 and name CA) (segid 3A4 and resid 267 and name CA)	17.22	0.37	0.37
30	assign (segid 3A4 and resid 256 and name CA) (segid 3A4 and resid 267 and name CB)	16.59	0.35	0.36
	assign (segid 3A4 and resid 256 and name CA) (segid 3A4 and resid 268 and name CA)	18.83	0.34	0.33
	assign (segid 3A4 and resid 256 and name CA) (segid 3A4 and resid 268 and name CB)	18.29	0.37	0.37
	assign (segid 3A4 and resid 256 and name CA) (segid 3A4 and resid 309 and name CA)	17.16	1.16	1.16
	assign (segid 3A4 and resid 256 and name CA) (segid 3A4 and resid 309 and name CB)	16.58	1.23	1.23
35	assign (segid 3A4 and resid 256 and name CA) (segid 3A4 and resid 312 and name CA)	17.32	1.06	1.06
	assign (segid 3A4 and resid 256 and name CA) (segid 3A4 and resid 312 and name CB)	16.52	1.13	1.12
	assign (segid 3A4 and resid 256 and name CA) (segid 3A4 and resid 313 and name CA)	15.45	0.95	0.95
	assign (segid 3A4 and resid 256 and name CA) (segid 3A4 and resid 313 and name CB)	15.09	0.99	0.99
	assign (segid 3A4 and resid 256 and name CA) (segid 3A4 and resid 316 and name CA)	16.48	0.81	0.81
40	assign (segid 3A4 and resid 256 and name CA) (segid 3A4 and resid 317 and name CA)	15.27	0.90	0.90
	assign (segid 3A4 and resid 256 and name CA) (segid 3A4 and resid 318 and name CA)	12.16	1.03	1.03
	assign (segid 3A4 and resid 256 and name CA) (segid 3A4 and resid 318 and name CB)	10.93	1.06	1.06
	assign (segid 3A4 and resid 256 and name CA) (segid 3A4 and resid 319 and name CA)	12.58	1.04	1.04
	assign (segid 3A4 and resid 256 and name CA) (segid 3A4 and resid 319 and name CB)	12.08	1.05	1.05
45	assign (segid 3A4 and resid 256 and name CA) (segid 3A4 and resid 347 and name CB)	17.81	0.57	0.58
	assign (segid 3A4 and resid 256 and name CA) (segid 3A4 and resid 383 and name CA)	15.62	0.59	0.60
	assign (segid 3A4 and resid 256 and name CA) (segid 3A4 and resid 384 and name CA)	14.36	0.55	0.56
	assign (segid 3A4 and resid 256 and name CA) (segid 3A4 and resid 384 and name CB)	14.45	0.60	0.60
	assign (segid 3A4 and resid 256 and name CA) (segid 3A4 and resid 385 and name CA)	16.92	0.45	0.45
50	assign (segid 3A4 and resid 256 and name CA) (segid 3A4 and resid 389 and name CA)	18.12	0.36	0.36
	assign (segid 3A4 and resid 256 and name CA) (segid 3A4 and resid 389 and name CB)	18.14	0.42	0.42
	assign (segid 3A4 and resid 256 and name CA) (segid 3A4 and resid 390 and name CA)	16.86	0.51	0.51
	assign (segid 3A4 and resid 256 and name CA) (segid 3A4 and resid 390 and name CB)	17.81	0.61	0.61
	assign (segid 3A4 and resid 256 and name CA) (segid 3A4 and resid 391 and name CA)	13.28	0.54	0.54
55	assign (segid 3A4 and resid 256 and name CA) (segid 3A4 and resid 391 and name CB)	12.45	0.58	0.57
	assign (segid 3A4 and resid 256 and name CA) (segid 3A4 and resid 392 and name CA)	13.51	0.56	0.57
	assign (segid 3A4 and resid 256 and name CA) (segid 3A4 and resid 392 and name CB)	13.50	0.62	0.61
	assign (segid 3A4 and resid 256 and name CA) (segid 3A4 and resid 393 and name CA)	10.77	0.43	0.43
	assign (segid 3A4 and resid 256 and name CA) (segid 3A4 and resid 394 and name CA)	12.62	0.50	0.50
60	assign (segid 3A4 and resid 256 and name CA) (segid 3A4 and resid 394 and name CB)	13.90	0.46	0.46
	assign (segid 3A4 and resid 256 and name CA) (segid 3A4 and resid 395 and name CA)	14.31	0.58	0.57
	assign (segid 3A4 and resid 256 and name CA) (segid 3A4 and resid 396 and name CA)	11.54	0.62	0.62
	assign (segid 3A4 and resid 256 and name CA) (segid 3A4 and resid 396 and name CB)	10.76	0.62	0.62
	assign (segid 3A4 and resid 256 and name CA) (segid 3A4 and resid 397 and name CA)	9.79	0.69	0.68
65	assign (segid 3A4 and resid 256 and name CA) (segid 3A4 and resid 397 and name CB)	9.54	0.68	0.69
	assign (segid 3A4 and resid 256 and name CA) (segid 3A4 and resid 398 and name CA)	13.30	0.73	0.74
	assign (segid 3A4 and resid 256 and name CA) (segid 3A4 and resid 398 and name CB)	14.50	0.74	0.74
	assign (segid 3A4 and resid 256 and name CA) (segid 3A4 and resid 399 and name CA)	14.13	0.73	0.73
	assign (segid 3A4 and resid 256 and name CA) (segid 3A4 and resid 399 and name CB)	14.27	0.79	0.78
70	assign (segid 3A4 and resid 256 and name CA) (segid 3A4 and resid 400 and name CA)	11.48	0.74	0.74
	assign (segid 3A4 and resid 256 and name CA) (segid 3A4 and resid 400 and name CB)	10.01	0.74	0.75
	assign (segid 3A4 and resid 256 and name CA) (segid 3A4 and resid 401 and name CA)	12.48	0.85	0.84
	assign (segid 3A4 and resid 256 and name CA) (segid 3A4 and resid 402 and name CA)	16.08	0.83	0.84
	assign (segid 3A4 and resid 256 and name CA) (segid 3A4 and resid 402 and name CB)	16.80	0.82	0.83
75	assign (segid 3A4 and resid 256 and name CA) (segid 3A4 and resid 403 and name CA)	16.18	0.72	0.73
	assign (segid 3A4 and resid 256 and name CA) (segid 3A4 and resid 403 and name CB)	15.62	0.69	0.70
	assign (segid 3A4 and resid 256 and name CA) (segid 3A4 and resid 404 and name CA)	14.71	0.81	0.83
	assign (segid 3A4 and resid 256 and name CA) (segid 3A4 and resid 404 and name CB)	13.34	0.88	0.89
	assign (segid 3A4 and resid 256 and name CA) (segid 3A4 and resid 405 and name CA)	16.96	1.08	1.08
80	assign (segid 3A4 and resid 256 and name CA) (segid 3A4 and resid 405 and name CB)	16.96	1.13	1.12
	assign (segid 3A4 and resid 256 and name CA) (segid 3A4 and resid 426 and name CA)	18.34	1.20	1.19
	assign (segid 3A4 and resid 256 and name CA) (segid 3A4 and resid 427 and name CA)	16.61	1.26	1.25

	assign (segid 3A4 and resid 256 and name CA)	(segid 3A4 and resid 128 and name CA)	17.19	0.95	0.95
	assign (segid 3A4 and resid 256 and name CA)	(segid 3A4 and resid 429 and name CA)	16.50	1.39	1.40
	assign (segid 3A4 and resid 256 and name CA)	(segid 3A4 and resid 430 and name CA)	16.33	1.83	1.83
	assign (segid 3A4 and resid 256 and name CA)	(segid 3A4 and resid 431 and name CA)	13.96	1.16	1.16
5	assign (segid 3A4 and resid 256 and name CA)	(segid 3A4 and resid 433 and name CA)	13.12	0.94	0.94
	assign (segid 3A4 and resid 256 and name CA)	(segid 3A4 and resid 434 and name CA)	12.46	0.62	0.62
	assign (segid 3A4 and resid 256 and name CA)	(segid 3A4 and resid 435 and name CA)	14.29	0.82	0.82
	assign (segid 3A4 and resid 256 and name CA)	(segid 3A4 and resid 436 and name CA)	14.96	1.72	1.73
	assign (segid 3A4 and resid 256 and name CA)	(segid 3A4 and resid 437 and name CA)	16.77	1.07	1.08
10	assign (segid 3A4 and resid 256 and name CA)	(segid HEM and resid 1 and name CMC)	6.39	0.60	0.61
	assign (segid 3A4 and resid 256 and name N)	(segid 3A4 and resid 256 and name C)	2.49	0.03	0.03
	assign (segid 3A4 and resid 256 and name N)	(segid 3A4 and resid 256 and name O)	1.45	0.01	0.00
	assign (segid 3A4 and resid 256 and name N)	(segid 3A4 and resid 257 and name C)	3.49	0.10	0.09
	assign (segid 3A4 and resid 256 and name N)	(segid 3A4 and resid 257 and name N)	4.93	0.09	0.09
15	assign (segid 3A4 and resid 256 and name N)	(segid 3A4 and resid 257 and name O)	4.33	0.01	0.01
	assign (segid 3A4 and resid 256 and name N)	(segid 3A4 and resid 257 and name N)	2.93	0.03	0.03
	assign (segid 3A4 and resid 256 and name N)	(segid 3A4 and resid 257 and name O)	5.96	0.11	0.12
	assign (segid 3A4 and resid 256 and name N)	(segid 3A4 and resid 258 and name C)	6.11	0.34	0.35
	assign (segid 3A4 and resid 256 and name N)	(segid 3A4 and resid 258 and name CA)	5.74	0.29	0.28
20	assign (segid 3A4 and resid 256 and name N)	(segid 3A4 and resid 258 and name CB)	5.80	0.38	0.39
	assign (segid 3A4 and resid 256 and name N)	(segid 3A4 and resid 258 and name N)	4.68	0.22	0.22
	assign (segid 3A4 and resid 256 and name N)	(segid 3A4 and resid 258 and name O)	7.27	0.28	0.29
	assign (segid 3A4 and resid 256 and name N)	(segid 3A4 and resid 259 and name C)	6.90	0.36	0.35
	assign (segid 3A4 and resid 256 and name N)	(segid 3A4 and resid 259 and name CA)	6.23	0.50	0.49
25	assign (segid 3A4 and resid 256 and name N)	(segid 3A4 and resid 259 and name CB)	5.77	0.63	0.64
	assign (segid 3A4 and resid 256 and name N)	(segid 3A4 and resid 259 and name N)	5.39	0.44	0.45
	assign (segid 3A4 and resid 256 and name N)	(segid 3A4 and resid 260 and name CA)	7.39	0.09	0.10
	assign (segid 3A4 and resid 256 and name N)	(segid 3A4 and resid 260 and name CB)	7.02	0.21	0.20
	assign (segid 3A4 and resid 256 and name N)	(segid 3A4 and resid 260 and name N)	6.39	0.21	0.22
30	assign (segid 3A4 and resid 256 and name N)	(segid HEM and resid 1 and name C1C)	6.27	0.56	0.56
	assign (segid 3A4 and resid 256 and name N)	(segid HEM and resid 1 and name C2C)	5.78	0.50	0.50
	assign (segid 3A4 and resid 256 and name N)	(segid HEM and resid 1 and name C3C)	6.08	0.47	0.46
	assign (segid 3A4 and resid 256 and name N)	(segid HEM and resid 1 and name C4C)	6.71	0.48	0.49
	assign (segid 3A4 and resid 256 and name N)	(segid HEM and resid 1 and name CAC)	6.24	0.42	0.42
35	assign (segid 3A4 and resid 256 and name N)	(segid HEM and resid 1 and name CBC)	6.54	0.30	0.30
	assign (segid 3A4 and resid 256 and name N)	(segid HEM and resid 1 and name CHC)	6.51	0.59	0.60
	assign (segid 3A4 and resid 256 and name N)	(segid HEM and resid 1 and name CMC)	5.60	0.47	0.47
	assign (segid 3A4 and resid 256 and name O)	(segid 3A4 and resid 257 and name C)	3.16	0.30	0.29
40	assign (segid 3A4 and resid 256 and name O)	(segid 3A4 and resid 257 and name N)	2.79	0.06	0.05
	assign (segid 3A4 and resid 256 and name O)	(segid 3A4 and resid 257 and name O)	2.25	0.01	0.01
	assign (segid 3A4 and resid 256 and name O)	(segid 3A4 and resid 258 and name C)	3.72	0.51	0.51
	assign (segid 3A4 and resid 256 and name O)	(segid 3A4 and resid 258 and name CA)	4.54	0.63	0.62
	assign (segid 3A4 and resid 256 and name O)	(segid 3A4 and resid 258 and name CB)	4.68	0.45	0.44
45	assign (segid 3A4 and resid 256 and name O)	(segid 3A4 and resid 258 and name N)	5.61	0.46	0.47
	assign (segid 3A4 and resid 256 and name O)	(segid 3A4 and resid 258 and name O)	3.65	0.34	0.34
	assign (segid 3A4 and resid 256 and name O)	(segid 3A4 and resid 259 and name C)	5.37	0.49	0.50
	assign (segid 3A4 and resid 256 and name O)	(segid 3A4 and resid 259 and name CA)	4.43	0.79	0.80
	assign (segid 3A4 and resid 256 and name O)	(segid 3A4 and resid 259 and name CB)	4.47	0.94	0.95
50	assign (segid 3A4 and resid 256 and name O)	(segid 3A4 and resid 259 and name N)	4.51	1.12	1.11
	assign (segid 3A4 and resid 256 and name O)	(segid 3A4 and resid 259 and name O)	3.90	0.85	0.86
	assign (segid 3A4 and resid 256 and name O)	(segid 3A4 and resid 260 and name C)	5.58	0.76	0.76
	assign (segid 3A4 and resid 256 and name O)	(segid 3A4 and resid 260 and name CA)	5.31	0.34	0.34
	assign (segid 3A4 and resid 256 and name O)	(segid 3A4 and resid 260 and name CB)	4.22	0.41	0.40
	assign (segid 3A4 and resid 256 and name O)	(segid 3A4 and resid 260 and name N)	3.71	0.15	0.16
55	assign (segid 3A4 and resid 256 and name O)	(segid 3A4 and resid 260 and name O)	3.52	0.68	0.68
	assign (segid 3A4 and resid 256 and name O)	(segid 3A4 and resid 261 and name CA)	6.43	0.31	0.30
	assign (segid 3A4 and resid 256 and name O)	(segid 3A4 and resid 261 and name N)	6.60	0.28	0.28
	assign (segid 3A4 and resid 256 and name O)	(segid 3A4 and resid 261 and name O)	5.29	0.33	0.33
	assign (segid 3A4 and resid 257 and name C)	(segid 3A4 and resid 257 and name O)	1.25	0.03	0.02
60	assign (segid 3A4 and resid 257 and name C)	(segid 3A4 and resid 258 and name C)	3.09	0.15	0.15
	assign (segid 3A4 and resid 257 and name C)	(segid 3A4 and resid 258 and name CA)	2.44	0.02	0.02
	assign (segid 3A4 and resid 257 and name C)	(segid 3A4 and resid 258 and name CB)	3.68	0.06	0.05
	assign (segid 3A4 and resid 257 and name C)	(segid 3A4 and resid 258 and name N)	1.32	0.01	0.01
	assign (segid 3A4 and resid 257 and name C)	(segid 3A4 and resid 258 and name O)	3.84	0.08	0.08
65	assign (segid 3A4 and resid 257 and name C)	(segid 3A4 and resid 259 and name C)	4.75	0.29	0.30
	assign (segid 3A4 and resid 257 and name C)	(segid 3A4 and resid 259 and name CA)	4.67	0.31	0.30
	assign (segid 3A4 and resid 257 and name C)	(segid 3A4 and resid 259 and name CB)	5.48	0.35	0.36
	assign (segid 3A4 and resid 257 and name C)	(segid 3A4 and resid 259 and name N)	3.46	0.26	0.26
	assign (segid 3A4 and resid 257 and name C)	(segid 3A4 and resid 259 and name O)	5.81	0.29	0.29
70	assign (segid 3A4 and resid 257 and name C)	(segid 3A4 and resid 260 and name C)	5.07	0.26	0.27
	assign (segid 3A4 and resid 257 and name C)	(segid 3A4 and resid 260 and name CA)	4.76	0.25	0.24
	assign (segid 3A4 and resid 257 and name C)	(segid 3A4 and resid 260 and name CB)	4.49	0.18	0.18
	assign (segid 3A4 and resid 257 and name C)	(segid 3A4 and resid 260 and name N)	4.03	0.30	0.31
	assign (segid 3A4 and resid 257 and name C)	(segid 3A4 and resid 260 and name O)	6.28	0.27	0.28
75	assign (segid 3A4 and resid 257 and name C)	(segid 3A4 and resid 261 and name C)	6.20	0.31	0.30
	assign (segid 3A4 and resid 257 and name C)	(segid 3A4 and resid 261 and name CA)	5.16	0.31	0.31
	assign (segid 3A4 and resid 257 and name C)	(segid 3A4 and resid 261 and name N)	4.30	0.29	0.29
	assign (segid 3A4 and resid 257 and name C)	(segid 3A4 and resid 262 and name CA)	7.32	0.25	0.26
	assign (segid 3A4 and resid 257 and name C)	(segid 3A4 and resid 262 and name CB)	7.34	0.22	0.21
80	assign (segid 3A4 and resid 257 and name C)	(segid 3A4 and resid 262 and name N)	6.06	0.27	0.28
	assign (segid 3A4 and resid 257 and name C)	(segid HEM and resid 1 and name C3B)	7.07	0.19	0.20
	assign (segid 3A4 and resid 257 and name C)	(segid HEM and resid 1 and name C4B)	7.29	0.22	0.22
	assign (segid 3A4 and resid 257 and name C)	(segid HEM and resid 1 and name CAB)	6.80	0.17	0.17

	assign (segid 3A4 and resid 257 and name C) (segid HEM and resid 1 and name CBB)	7.05	0.33	0.32
	assign (segid 3A4 and resid 257 and name C) (segid HEM and resid 1 and name CHC)	7.28	0.21	0.21
	assign (segid 3A4 and resid 257 and name CA) (segid 3A4 and resid 257 and name C)	1.51	0.02	0.02
	assign (segid 3A4 and resid 257 and name CA) (segid 3A4 and resid 257 and name O)	2.37	0.03	0.03
5	assign (segid 3A4 and resid 257 and name CA) (segid 3A4 and resid 258 and name C)	4.48	0.13	0.12
	assign (segid 3A4 and resid 257 and name CA) (segid 3A4 and resid 258 and name CA)	3.81	0.02	0.02
	assign (segid 3A4 and resid 257 and name CA) (segid 3A4 and resid 258 and name CB)	4.83	0.03	0.04
	assign (segid 3A4 and resid 257 and name CA) (segid 3A4 and resid 258 and name N)	2.44	0.02	0.02
	assign (segid 3A4 and resid 257 and name CA) (segid 3A4 and resid 258 and name O)	5.28	0.08	0.08
10	assign (segid 3A4 and resid 257 and name CA) (segid 3A4 and resid 259 and name C)	5.71	0.30	0.29
	assign (segid 3A4 and resid 257 and name CA) (segid 3A4 and resid 259 and name CA)	5.69	0.32	0.32
	assign (segid 3A4 and resid 257 and name CA) (segid 3A4 and resid 259 and name CB)	6.24	0.42	0.42
	assign (segid 3A4 and resid 257 and name CA) (segid 3A4 and resid 259 and name N)	4.58	0.27	0.26
	assign (segid 3A4 and resid 257 and name CA) (segid 3A4 and resid 259 and name O)	6.82	0.30	0.29
15	assign (segid 3A4 and resid 257 and name CA) (segid 3A4 and resid 260 and name C)	5.86	0.26	0.26
	assign (segid 3A4 and resid 257 and name CA) (segid 3A4 and resid 260 and name CA)	5.32	0.22	0.22
	assign (segid 3A4 and resid 257 and name CA) (segid 3A4 and resid 260 and name CB)	4.66	0.12	0.11
	assign (segid 3A4 and resid 257 and name CA) (segid 3A4 and resid 260 and name N)	4.78	0.30	0.30
	assign (segid 3A4 and resid 257 and name CA) (segid 3A4 and resid 260 and name O)	7.05	0.27	0.27
20	assign (segid 3A4 and resid 257 and name CA) (segid 3A4 and resid 261 and name C)	7.39	0.32	0.31
	assign (segid 3A4 and resid 257 and name CA) (segid 3A4 and resid 261 and name CA)	6.21	0.34	0.33
	assign (segid 3A4 and resid 257 and name CA) (segid 3A4 and resid 261 and name N)	5.26	0.30	0.30
	assign (segid 3A4 and resid 257 and name CA) (segid 3A4 and resid 262 and name CA)	8.67	0.25	0.25
	assign (segid 3A4 and resid 257 and name CA) (segid 3A4 and resid 262 and name CB)	8.72	0.22	0.21
25	assign (segid 3A4 and resid 257 and name CA) (segid 3A4 and resid 262 and name N)	7.36	0.27	0.28
	assign (segid 3A4 and resid 257 and name CA) (segid 3A4 and resid 263 and name CA)	10.24	0.32	0.31
	assign (segid 3A4 and resid 257 and name CA) (segid 3A4 and resid 263 and name CB)	9.93	0.33	0.33
	assign (segid 3A4 and resid 257 and name CA) (segid 3A4 and resid 264 and name CA)	10.81	0.45	0.44
	assign (segid 3A4 and resid 257 and name CA) (segid 3A4 and resid 265 and name CA)	12.23	0.43	0.43
30	assign (segid 3A4 and resid 257 and name CA) (segid 3A4 and resid 266 and name CA)	14.26	0.36	0.35
	assign (segid 3A4 and resid 257 and name CA) (segid 3A4 and resid 267 and name CA)	15.77	0.34	0.35
	assign (segid 3A4 and resid 257 and name CA) (segid 3A4 and resid 267 and name CB)	15.26	0.38	0.37
	assign (segid 3A4 and resid 257 and name CA) (segid 3A4 and resid 268 and name CA)	16.71	0.40	0.41
	assign (segid 3A4 and resid 257 and name CA) (segid 3A4 and resid 268 and name CB)	15.94	0.45	0.45
35	assign (segid 3A4 and resid 257 and name CA) (segid 3A4 and resid 269 and name CA)	18.40	0.41	0.42
	assign (segid 3A4 and resid 257 and name CA) (segid 3A4 and resid 309 and name CA)	16.66	1.00	0.99
	assign (segid 3A4 and resid 257 and name CA) (segid 3A4 and resid 309 and name CB)	16.40	1.04	1.04
	assign (segid 3A4 and resid 257 and name CA) (segid 3A4 and resid 310 and name CA)	17.86	0.89	0.90
	assign (segid 3A4 and resid 257 and name CA) (segid 3A4 and resid 312 and name CA)	15.74	0.96	0.96
40	assign (segid 3A4 and resid 257 and name CA) (segid 3A4 and resid 312 and name CB)	15.10	1.01	1.02
	assign (segid 3A4 and resid 257 and name CA) (segid 3A4 and resid 313 and name CA)	13.93	0.80	0.81
	assign (segid 3A4 and resid 257 and name CA) (segid 3A4 and resid 313 and name CB)	13.90	0.81	0.80
	assign (segid 3A4 and resid 257 and name CA) (segid 3A4 and resid 314 and name CA)	17.02	0.68	0.68
	assign (segid 3A4 and resid 257 and name CA) (segid 3A4 and resid 314 and name CB)	18.45	0.69	0.69
45	assign (segid 3A4 and resid 257 and name CA) (segid 3A4 and resid 315 and name CA)	17.32	0.73	0.73
	assign (segid 3A4 and resid 257 and name CA) (segid 3A4 and resid 315 and name CB)	17.87	0.82	0.82
	assign (segid 3A4 and resid 257 and name CA) (segid 3A4 and resid 316 and name CA)	13.89	0.81	0.81
	assign (segid 3A4 and resid 257 and name CA) (segid 3A4 and resid 317 and name CA)	12.81	0.78	0.78
	assign (segid 3A4 and resid 257 and name CA) (segid 3A4 and resid 318 and name CA)	9.34	0.89	0.89
50	assign (segid 3A4 and resid 257 and name CA) (segid 3A4 and resid 318 and name CB)	8.23	0.94	0.93
	assign (segid 3A4 and resid 257 and name CA) (segid 3A4 and resid 319 and name CA)	10.04	0.75	0.74
	assign (segid 3A4 and resid 257 and name CA) (segid 3A4 and resid 319 and name CB)	9.91	0.63	0.64
	assign (segid 3A4 and resid 257 and name CA) (segid 3A4 and resid 322 and name CA)	18.48	0.70	0.70
	assign (segid 3A4 and resid 257 and name CA) (segid 3A4 and resid 347 and name CA)	17.00	0.80	0.80
55	assign (segid 3A4 and resid 257 and name CA) (segid 3A4 and resid 347 and name CB)	15.73	0.81	0.82
	assign (segid 3A4 and resid 257 and name CA) (segid 3A4 and resid 382 and name CA)	16.84	0.85	0.85
	assign (segid 3A4 and resid 257 and name CA) (segid 3A4 and resid 382 and name CB)	17.83	0.32	0.31
	assign (segid 3A4 and resid 257 and name CA) (segid 3A4 and resid 382 and name N)	18.54	0.34	0.34
60	assign (segid 3A4 and resid 257 and name CA) (segid 3A4 and resid 383 and name CA)	14.24	0.35	0.35
	assign (segid 3A4 and resid 257 and name CA) (segid 3A4 and resid 384 and name CA)	13.77	0.23	0.23
	assign (segid 3A4 and resid 257 and name CA) (segid 3A4 and resid 384 and name CB)	14.20	0.20	0.20
	assign (segid 3A4 and resid 257 and name CA) (segid 3A4 and resid 385 and name CA)	16.10	0.29	0.29
	assign (segid 3A4 and resid 257 and name CA) (segid 3A4 and resid 389 and name CA)	18.29	0.44	0.43
	assign (segid 3A4 and resid 257 and name CA) (segid 3A4 and resid 389 and name CB)	18.08	0.62	0.62
65	assign (segid 3A4 and resid 257 and name CA) (segid 3A4 and resid 390 and name CA)	17.02	0.26	0.25
	assign (segid 3A4 and resid 257 and name CA) (segid 3A4 and resid 390 and name CB)	18.04	0.30	0.30
	assign (segid 3A4 and resid 257 and name CA) (segid 3A4 and resid 391 and name CA)	13.80	0.26	0.26
	assign (segid 3A4 and resid 257 and name CA) (segid 3A4 and resid 391 and name CB)	12.82	0.23	0.23
	assign (segid 3A4 and resid 257 and name CA) (segid 3A4 and resid 392 and name CA)	14.97	0.41	0.41
70	assign (segid 3A4 and resid 257 and name CA) (segid 3A4 and resid 392 and name CB)	15.12	0.49	0.50
	assign (segid 3A4 and resid 257 and name CA) (segid 3A4 and resid 393 and name CA)	12.56	0.43	0.43
	assign (segid 3A4 and resid 257 and name CA) (segid 3A4 and resid 394 and name CA)	13.70	0.32	0.32
	assign (segid 3A4 and resid 257 and name CA) (segid 3A4 and resid 394 and name CB)	14.76	0.33	0.34
	assign (segid 3A4 and resid 257 and name CA) (segid 3A4 and resid 395 and name CA)	15.98	0.37	0.38
75	assign (segid 3A4 and resid 257 and name CA) (segid 3A4 and resid 396 and name CA)	13.77	0.48	0.48
	assign (segid 3A4 and resid 257 and name CA) (segid 3A4 and resid 396 and name CB)	13.25	0.54	0.55
	assign (segid 3A4 and resid 257 and name CA) (segid 3A4 and resid 397 and name CA)	11.18	0.37	0.38
	assign (segid 3A4 and resid 257 and name CA) (segid 3A4 and resid 397 and name CB)	10.58	0.36	0.37
	assign (segid 3A4 and resid 257 and name CA) (segid 3A4 and resid 398 and name CA)	14.30	0.42	0.41
80	assign (segid 3A4 and resid 257 and name CA) (segid 3A4 and resid 398 and name CB)	15.43	0.42	0.42
	assign (segid 3A4 and resid 257 and name CA) (segid 3A4 and resid 399 and name CA)	15.84	0.43	0.44
	assign (segid 3A4 and resid 257 and name CA) (segid 3A4 and resid 399 and name CB)	16.28	0.48	0.49
	assign (segid 3A4 and resid 257 and name CA) (segid 3A4 and resid 400 and name CA)	13.22	0.47	0.47

5	assign	(segid 3A4 and resid 257 and name CA)	(segid 3A4 and resid 400 and name CB)	11.88	0.52	0.51
	assign	(segid 3A4 and resid 257 and name CA)	(segid 3A4 and resid 401 and name CA)	13.16	0.56	0.57
	assign	(segid 3A4 and resid 257 and name CA)	(segid 3A4 and resid 402 and name CA)	16.94	0.57	0.57
	assign	(segid 3A4 and resid 257 and name CA)	(segid 3A4 and resid 402 and name CB)	17.78	0.55	0.54
	assign	(segid 3A4 and resid 257 and name CA)	(segid 3A4 and resid 403 and name CA)	17.61	0.44	0.43
	assign	(segid 3A4 and resid 257 and name CA)	(segid 3A4 and resid 403 and name CB)	17.35	0.41	0.40
	assign	(segid 3A4 and resid 257 and name CA)	(segid 3A4 and resid 404 and name CA)	15.70	0.55	0.55
	assign	(segid 3A4 and resid 257 and name CA)	(segid 3A4 and resid 404 and name CB)	14.23	0.57	0.56
	assign	(segid 3A4 and resid 257 and name CA)	(segid 3A4 and resid 405 and name CA)	17.26	0.91	0.91
10	assign	(segid 3A4 and resid 257 and name CA)	(segid 3A4 and resid 405 and name CB)	17.06	0.95	0.94
	assign	(segid 3A4 and resid 257 and name CA)	(segid 3A4 and resid 425 and name CA)	17.04	1.30	1.31
	assign	(segid 3A4 and resid 257 and name CA)	(segid 3A4 and resid 426 and name CA)	14.91	1.33	1.33
	assign	(segid 3A4 and resid 257 and name CA)	(segid 3A4 and resid 427 and name CA)	12.98	1.28	1.28
	assign	(segid 3A4 and resid 257 and name CA)	(segid 3A4 and resid 428 and name CA)	13.52	0.89	0.90
15	assign	(segid 3A4 and resid 257 and name CA)	(segid 3A4 and resid 429 and name CA)	12.86	1.42	1.42
	assign	(segid 3A4 and resid 257 and name CA)	(segid 3A4 and resid 430 and name CA)	12.92	1.80	1.80
	assign	(segid 3A4 and resid 257 and name CA)	(segid 3A4 and resid 431 and name CA)	10.80	1.01	1.01
	assign	(segid 3A4 and resid 257 and name CA)	(segid 3A4 and resid 433 and name CA)	9.55	1.05	1.05
	assign	(segid 3A4 and resid 257 and name CA)	(segid 3A4 and resid 434 and name CA)	9.01	0.60	0.60
20	assign	(segid 3A4 and resid 257 and name CA)	(segid 3A4 and resid 435 and name CA)	11.13	0.83	0.84
	assign	(segid 3A4 and resid 257 and name CA)	(segid 3A4 and resid 436 and name CA)	11.96	1.70	1.71
	assign	(segid 3A4 and resid 257 and name CA)	(segid 3A4 and resid 437 and name CA)	14.24	1.05	1.06
	assign	(segid 3A4 and resid 257 and name CA)	(segid 3A4 and resid 438 and name CA)	15.73	0.96	0.95
	assign	(segid 3A4 and resid 257 and name CA)	(segid 3A4 and resid 439 and name CA)	18.64	0.75	0.76
25	assign	(segid 3A4 and resid 257 and name N)	(segid 3A4 and resid 257 and name C)	2.50	0.04	0.04
	assign	(segid 3A4 and resid 257 and name N)	(segid 3A4 and resid 257 and name CA)	1.46	0.02	0.01
	assign	(segid 3A4 and resid 257 and name N)	(segid 3A4 and resid 257 and name O)	3.51	0.06	0.06
	assign	(segid 3A4 and resid 257 and name N)	(segid 3A4 and resid 258 and name C)	4.90	0.18	0.17
	assign	(segid 3A4 and resid 257 and name N)	(segid 3A4 and resid 258 and name CA)	4.32	0.10	0.11
30	assign	(segid 3A4 and resid 257 and name N)	(segid 3A4 and resid 258 and name CB)	5.04	0.11	0.11
	assign	(segid 3A4 and resid 257 and name N)	(segid 3A4 and resid 258 and name N)	2.92	0.11	0.10
	assign	(segid 3A4 and resid 257 and name N)	(segid 3A4 and resid 258 and name O)	5.89	0.10	0.10
	assign	(segid 3A4 and resid 257 and name N)	(segid 3A4 and resid 259 and name C)	5.92	0.30	0.31
	assign	(segid 3A4 and resid 257 and name N)	(segid 3A4 and resid 259 and name CA)	5.70	0.37	0.37
35	assign	(segid 3A4 and resid 257 and name N)	(segid 3A4 and resid 259 and name CB)	5.90	0.49	0.50
	assign	(segid 3A4 and resid 257 and name N)	(segid 3A4 and resid 259 and name N)	4.65	0.32	0.31
	assign	(segid 3A4 and resid 257 and name N)	(segid 3A4 and resid 259 and name O)	7.11	0.30	0.31
	assign	(segid 3A4 and resid 257 and name N)	(segid 3A4 and resid 260 and name C)	6.60	0.20	0.20
	assign	(segid 3A4 and resid 257 and name N)	(segid 3A4 and resid 260 and name CA)	5.79	0.16	0.15
40	assign	(segid 3A4 and resid 257 and name N)	(segid 3A4 and resid 260 and name CB)	5.14	0.03	0.04
	assign	(segid 3A4 and resid 257 and name N)	(segid 3A4 and resid 260 and name N)	5.07	0.27	0.26
	assign	(segid 3A4 and resid 257 and name N)	(segid 3A4 and resid 261 and name CA)	7.30	0.28	0.27
	assign	(segid 3A4 and resid 257 and name N)	(segid 3A4 and resid 261 and name N)	6.20	0.24	0.24
	assign	(segid 3A4 and resid 257 and name N)	(segid HEM and resid 1 and name CHC)	7.57	0.13	0.14
45	assign	(segid 3A4 and resid 257 and name O)	(segid 3A4 and resid 258 and name C)	3.11	0.31	0.30
	assign	(segid 3A4 and resid 257 and name O)	(segid 3A4 and resid 258 and name CA)	2.76	0.03	0.04
	assign	(segid 3A4 and resid 257 and name O)	(segid 3A4 and resid 258 and name CB)	4.16	0.19	0.18
	assign	(segid 3A4 and resid 257 and name O)	(segid 3A4 and resid 258 and name N)	2.23	0.02	0.03
	assign	(

	assign (segid 3A4 and resid 258 and name C)	(segid 3A4 and resid 262 and name CA)	5.07	0.07	0.06
	assign (segid 3A4 and resid 258 and name C)	(segid 3A4 and resid 262 and name CB)	1.64	0.05	0.05
	assign (segid 3A4 and resid 258 and name C)	(segid 3A4 and resid 262 and name N)	4.20	0.10	0.09
	assign (segid 3A4 and resid 258 and name C)	(segid 3A4 and resid 262 and name O)	7.33	0.07	0.07
5	assign (segid 3A4 and resid 258 and name C)	(segid 3A4 and resid 263 and name CA)	7.42	0.08	0.07
	assign (segid 3A4 and resid 258 and name C)	(segid 3A4 and resid 263 and name CB)	7.49	0.09	0.09
	assign (segid 3A4 and resid 258 and name C)	(segid 3A4 and resid 263 and name CG)	7.18	0.25	0.25
	assign (segid 3A4 and resid 258 and name C)	(segid 3A4 and resid 263 and name N)	6.10	0.06	0.07
	assign (segid 3A4 and resid 258 and name C)	(segid 3A4 and resid 318 and name CB)	5.53	0.82	0.81
10	assign (segid 3A4 and resid 258 and name C)	(segid 3A4 and resid 397 and name CB)	7.12	0.37	0.37
	assign (segid 3A4 and resid 258 and name C)	(segid HEM and resid 1 and name C1B)	6.36	0.23	0.23
	assign (segid 3A4 and resid 258 and name C)	(segid HEM and resid 1 and name C1C)	6.61	0.21	0.21
	assign (segid 3A4 and resid 258 and name C)	(segid HEM and resid 1 and name C2B)	5.45	0.23	0.23
	assign (segid 3A4 and resid 258 and name C)	(segid HEM and resid 1 and name C2C)	7.12	0.20	0.20
15	assign (segid 3A4 and resid 258 and name C)	(segid HEM and resid 1 and name C3B)	4.80	0.21	0.21
	assign (segid 3A4 and resid 258 and name C)	(segid HEM and resid 1 and name C4B)	5.45	0.22	0.22
	assign (segid 3A4 and resid 258 and name C)	(segid HEM and resid 1 and name CAB)	4.14	0.20	0.20
	assign (segid 3A4 and resid 258 and name C)	(segid HEM and resid 1 and name CBB)	4.11	0.31	0.31
	assign (segid 3A4 and resid 258 and name C)	(segid HEM and resid 1 and name CHB)	7.42	0.21	0.21
20	assign (segid 3A4 and resid 258 and name C)	(segid HEM and resid 1 and name CHC)	5.59	0.20	0.20
	assign (segid 3A4 and resid 258 and name C)	(segid HEM and resid 1 and name CMB)	5.73	0.29	0.28
	assign (segid 3A4 and resid 258 and name C)	(segid HEM and resid 1 and name CMC)	6.86	0.21	0.20
	assign (segid 3A4 and resid 258 and name C)	(segid HEM and resid 1 and name NB)	6.37	0.23	0.24
	assign (segid 3A4 and resid 258 and name CA)	(segid 3A4 and resid 258 and name C)	1.53	0.01	0.01
25	assign (segid 3A4 and resid 258 and name CA)	(segid 3A4 and resid 258 and name CB)	1.55	0.02	0.01
	assign (segid 3A4 and resid 258 and name CA)	(segid 3A4 and resid 258 and name O)	2.40	0.02	0.01
	assign (segid 3A4 and resid 258 and name CA)	(segid 3A4 and resid 259 and name C)	4.46	0.05	0.04
	assign (segid 3A4 and resid 258 and name CA)	(segid 3A4 and resid 259 and name CA)	3.82	0.01	0.01
	assign (segid 3A4 and resid 258 and name CA)	(segid 3A4 and resid 259 and name CB)	4.86	0.02	0.01
30	assign (segid 3A4 and resid 258 and name CA)	(segid 3A4 and resid 259 and name N)	2.44	0.02	0.03
	assign (segid 3A4 and resid 258 and name CA)	(segid 3A4 and resid 259 and name O)	5.39	0.04	0.03
	assign (segid 3A4 and resid 258 and name CA)	(segid 3A4 and resid 260 and name C)	5.60	0.08	0.08
	assign (segid 3A4 and resid 258 and name CA)	(segid 3A4 and resid 260 and name CA)	5.52	0.13	0.13
35	assign (segid 3A4 and resid 258 and name CA)	(segid 3A4 and resid 260 and name CB)	5.88	0.27	0.26
	assign (segid 3A4 and resid 258 and name CA)	(segid 3A4 and resid 260 and name N)	4.42	0.11	0.12
	assign (segid 3A4 and resid 258 and name CA)	(segid 3A4 and resid 260 and name O)	6.72	0.07	0.08
	assign (segid 3A4 and resid 258 and name CA)	(segid 3A4 and resid 261 and name C)	5.82	0.13	0.14
	assign (segid 3A4 and resid 258 and name CA)	(segid 3A4 and resid 261 and name CA)	5.31	0.16	0.15
	assign (segid 3A4 and resid 258 and name CA)	(segid 3A4 and resid 261 and name N)	4.71	0.09	0.10
40	assign (segid 3A4 and resid 258 and name CA)	(segid 3A4 and resid 261 and name O)	7.00	0.17	0.16
	assign (segid 3A4 and resid 258 and name CA)	(segid 3A4 and resid 262 and name C)	7.48	0.09	0.09
	assign (segid 3A4 and resid 258 and name CA)	(segid 3A4 and resid 262 and name CA)	6.25	0.09	0.09
	assign (segid 3A4 and resid 258 and name CA)	(segid 3A4 and resid 262 and name CB)	5.90	0.08	0.08
	assign (segid 3A4 and resid 258 and name CA)	(segid 3A4 and resid 262 and name N)	5.29	0.12	0.12
45	assign (segid 3A4 and resid 258 and name CA)	(segid 3A4 and resid 263 and name CA)	8.83	0.07	0.07
	assign (segid 3A4 and resid 258 and name CA)	(segid 3A4 and resid 263 and name CB)	8.93	0.08	0.08
	assign (segid 3A4 and resid 258 and name CA)	(segid 3A4 and resid 263 and name N)	7.49	0.07	0.08
	assign (segid 3A4 and resid 258 and name CA)	(segid 3A4 and resid 264 and name CA)	10.11	0.18	0.18
	assign (segid 3A4 and resid 258 and name CA)	(segid 3A4 and resid 265 and name CA)	10.55	0.34	0.34
50	assign (segid 3A4 and resid 258 and name CA)	(segid 3A4 and resid 266 and name CA)	12.20	0.24	0.23
	assign (segid 3A4 and resid 258 and name CA)	(segid 3A4 and resid 267 and name CA)	14.49	0.16	0.16
	assign (segid 3A4 and resid 258 and name CA)	(segid 3A4 and resid 267 and name CB)	14.30	0.17	0.18
	assign (segid 3A4 and resid 258 and name CA)	(segid 3A4 and resid 268 and name CA)	15.48	0.24	0.25
	assign (segid 3A4 and resid 258 and name CA)	(segid 3A4 and resid 268 and name CB)	14.77	0.32	0.31
55	assign (segid 3A4 and resid 258 and name CA)	(segid 3A4 and resid 269 and name CA)	16.45	0.40	0.40
	assign (segid 3A4 and resid 258 and name CA)	(segid 3A4 and resid 270 and name CA)	18.40	0.19	0.19
	assign (segid 3A4 and resid 258 and name CA)	(segid 3A4 and resid 270 and name CB)	18.04	0.14	0.15
	assign (segid 3A4 and resid 258 and name CA)	(segid 3A4 and resid 271 and name CB)	19.47	0.21	0.21
	assign (segid 3A4 and resid 258 and name CA)	(segid 3A4 and resid 306 and name CA)	17.61	0.80	0.79
60	assign (segid 3A4 and resid 258 and name CA)	(segid 3A4 and resid 307 and name CA)	18.64	0.83	0.82
	assign (segid 3A4 and resid 258 and name CA)	(segid 3A4 and resid 308 and name CA)	16.97	0.77	0.78
	assign (segid 3A4 and resid 258 and name CA)	(segid 3A4 and resid 308 and name CB)	17.35	0.77	0.77
	assign (segid 3A4 and resid 258 and name CA)	(segid 3A4 and resid 309 and name CA)	13.54	0.80	0.80
	assign (segid 3A4 and resid 258 and name CA)	(segid 3A4 and resid 309 and name CB)	13.36	0.84	0.83
65	assign (segid 3A4 and resid 258 and name CA)	(segid 3A4 and resid 310 and name CA)	14.34	0.81	0.80
	assign (segid 3A4 and resid 258 and name CA)	(segid 3A4 and resid 310 and name CB)	15.62	0.82	0.81
	assign (segid 3A4 and resid 258 and name CA)	(segid 3A4 and resid 311 and name CA)	15.53	0.77	0.76
	assign (segid 3A4 and resid 258 and name CA)	(segid 3A4 and resid 311 and name CB)	16.79	0.78	0.79
	assign (segid 3A4 and resid 258 and name CA)	(segid 3A4 and resid 312 and name CA)	12.59	0.78	0.78
70	assign (segid 3A4 and resid 258 and name CA)	(segid 3A4 and resid 312 and name CB)	12.10	0.80	0.81
	assign (segid 3A4 and resid 258 and name CA)	(segid 3A4 and resid 313 and name CA)	10.37	0.74	0.73
	assign (segid 3A4 and resid 258 and name CA)	(segid 3A4 and resid 313 and name CB)	10.23	0.76	0.76
	assign (segid 3A4 and resid 258 and name CA)	(segid 3A4 and resid 314 and name CA)	13.45	0.65	0.65
	assign (segid 3A4 and resid 258 and name CA)	(segid 3A4 and resid 314 and name CB)	14.87	0.66	0.65
75	assign (segid 3A4 and resid 258 and name CA)	(segid 3A4 and resid 315 and name CA)	14.15	0.61	0.61
	assign (segid 3A4 and resid 258 and name CA)	(segid 3A4 and resid 315 and name CB)	14.80	0.68	0.69
	assign (segid 3A4 and resid 258 and name CA)	(segid 3A4 and resid 316 and name CA)	10.98	0.67	0.67
	assign (segid 3A4 and resid 258 and name CA)	(segid 3A4 and resid 317 and name CA)	9.56	0.74	0.74
	assign (segid 3A4 and resid 258 and name CA)	(segid 3A4 and resid 318 and name CA)	6.52	0.91	0.90
80	assign (segid 3A4 and resid 258 and name CA)	(segid 3A4 and resid 318 and name CB)	5.28	0.95	0.95
	assign (segid 3A4 and resid 258 and name CA)	(segid 3A4 and resid 318 and name O)	6.61	0.83	0.84
	assign (segid 3A4 and resid 258 and name CA)	(segid 3A4 and resid 319 and name CA)	7.49	0.79	0.78
	assign (segid 3A4 and resid 258 and name CA)	(segid 3A4 and resid 319 and name CB)	7.22	0.69	0.70

	assign (segid 3A4 and resid 258 and name CA) (segid 3A4 and resid 322 and name CA)	16.99	0.49	0.49
	assign (segid 3A4 and resid 258 and name CA) (segid 3A4 and resid 344 and name CA)	18.71	0.23	0.22
	assign (segid 3A4 and resid 258 and name CA) (segid 3A4 and resid 344 and name CB)	18.61	0.22	0.22
	assign (segid 3A4 and resid 258 and name CA) (segid 3A4 and resid 345 and name CA)	17.52	0.48	0.47
5	assign (segid 3A4 and resid 258 and name CA) (segid 3A4 and resid 345 and name CB)	17.37	0.69	0.69
	assign (segid 3A4 and resid 258 and name CA) (segid 3A4 and resid 346 and name CA)	16.02	0.65	0.65
	assign (segid 3A4 and resid 258 and name CA) (segid 3A4 and resid 346 and name CB)	16.93	0.75	0.75
	assign (segid 3A4 and resid 258 and name CA) (segid 3A4 and resid 347 and name CA)	13.96	0.64	0.64
	assign (segid 3A4 and resid 258 and name CA) (segid 3A4 and resid 347 and name CB)	12.65	0.67	0.67
10	assign (segid 3A4 and resid 258 and name CA) (segid 3A4 and resid 348 and name CA)	13.89	0.70	0.70
	assign (segid 3A4 and resid 258 and name CA) (segid 3A4 and resid 349 and name CA)	17.64	0.64	0.64
	assign (segid 3A4 and resid 258 and name CA) (segid 3A4 and resid 349 and name CB)	18.46	0.62	0.62
	assign (segid 3A4 and resid 258 and name CA) (segid 3A4 and resid 350 and name CA)	18.15	0.42	0.42
	assign (segid 3A4 and resid 258 and name CA) (segid 3A4 and resid 350 and name CB)	17.65	0.47	0.47
15	assign (segid 3A4 and resid 258 and name CA) (segid 3A4 and resid 351 and name CA)	16.70	0.50	0.50
	assign (segid 3A4 and resid 258 and name CA) (segid 3A4 and resid 352 and name CA)	19.06	0.35	0.34
	assign (segid 3A4 and resid 258 and name CA) (segid 3A4 and resid 352 and name CB)	18.73	0.41	0.41
	assign (segid 3A4 and resid 258 and name CA) (segid 3A4 and resid 363 and name CA)	18.79	0.60	0.59
	assign (segid 3A4 and resid 258 and name CA) (segid 3A4 and resid 381 and name CA)	16.13	0.45	0.46
20	assign (segid 3A4 and resid 258 and name CA) (segid 3A4 and resid 382 and name CA)	14.24	0.34	0.34
	assign (segid 3A4 and resid 258 and name CA) (segid 3A4 and resid 382 and name CB)	15.05	0.35	0.35
	assign (segid 3A4 and resid 258 and name CA) (segid 3A4 and resid 383 and name CA)	10.58	0.37	0.38
	assign (segid 3A4 and resid 258 and name CA) (segid 3A4 and resid 384 and name CA)	10.32	0.30	0.30
	assign (segid 3A4 and resid 258 and name CA) (segid 3A4 and resid 384 and name CB)	10.75	0.28	0.28
25	assign (segid 3A4 and resid 258 and name CA) (segid 3A4 and resid 385 and name CA)	12.94	0.29	0.28
	assign (segid 3A4 and resid 258 and name CA) (segid 3A4 and resid 386 and name CA)	16.54	0.28	0.28
	assign (segid 3A4 and resid 258 and name CA) (segid 3A4 and resid 389 and name CA)	16.10	0.36	0.35
	assign (segid 3A4 and resid 258 and name CA) (segid 3A4 and resid 389 and name CB)	16.01	0.50	0.50
	assign (segid 3A4 and resid 258 and name CA) (segid 3A4 and resid 390 and name CA)	14.28	0.33	0.33
30	assign (segid 3A4 and resid 258 and name CA) (segid 3A4 and resid 390 and name CB)	15.16	0.41	0.42
	assign (segid 3A4 and resid 258 and name CA) (segid 3A4 and resid 391 and name CA)	11.20	0.34	0.34
	assign (segid 3A4 and resid 258 and name CA) (segid 3A4 and resid 391 and name CB)	10.00	0.34	0.33
	assign (segid 3A4 and resid 258 and name CA) (segid 3A4 and resid 392 and name CA)	12.93	0.39	0.39
	assign (segid 3A4 and resid 258 and name CA) (segid 3A4 and resid 392 and name CB)	13.42	0.42	0.42
35	assign (segid 3A4 and resid 258 and name CA) (segid 3A4 and resid 393 and name CA)	10.57	0.50	0.49
	assign (segid 3A4 and resid 258 and name CA) (segid 3A4 and resid 394 and name CA)	10.83	0.41	0.41
	assign (segid 3A4 and resid 258 and name CA) (segid 3A4 and resid 394 and name CB)	11.74	0.45	0.45
	assign (segid 3A4 and resid 258 and name CA) (segid 3A4 and resid 395 and name CA)	13.45	0.39	0.40
	assign (segid 3A4 and resid 258 and name CA) (segid 3A4 and resid 396 and name CA)	11.91	0.51	0.51
40	assign (segid 3A4 and resid 258 and name CA) (segid 3A4 and resid 396 and name CB)	11.70	0.60	0.61
	assign (segid 3A4 and resid 258 and name CA) (segid 3A4 and resid 397 and name CA)	8.78	0.37	0.38
	assign (segid 3A4 and resid 258 and name CA) (segid 3A4 and resid 397 and name CB)	7.87	0.36	0.37
	assign (segid 3A4 and resid 258 and name CA) (segid 3A4 and resid 398 and name CA)	11.51	0.30	0.30
	assign (segid 3A4 and resid 258 and name CA) (segid 3A4 and resid 398 and name CB)	12.48	0.33	0.34
45	assign (segid 3A4 and resid 258 and name CA) (segid 3A4 and resid 399 and name CA)	13.73	0.33	0.34
	assign (segid 3A4 and resid 258 and name CA) (segid 3A4 and resid 399 and name CB)	14.34	0.37	0.38
	assign (segid 3A4 and resid 258 and name CA) (segid 3A4 and resid 400 and name CA)	11.71	0.43	0.42
	assign (segid 3A4 and resid 258 and name CA) (segid 3A4 and resid 400 and name CB)	10.53	0.53	0.53
50	assign (segid 3A4 and resid 258 and name CA) (segid 3A4 and resid 401 and name CA)	11.07	0.29	0.29
	assign (segid 3A4 and resid 258 and name CA) (segid 3A4 and resid 402 and name CA)	14.72	0.30	0.31
	assign (segid 3A4 and resid 258 and name CA) (segid 3A4 and resid 402 and name CB)	15.42	0.31	0.31
	assign (segid 3A4 and resid 258 and name CA) (segid 3A4 and resid 403 and name CA)	16.11	0.23	0.22
	assign (segid 3A4 and resid 258 and name CA) (segid 3A4 and resid 403 and name CB)	16.02	0.24	0.24
	assign (segid 3A4 and resid 258 and name CA) (segid 3A4 and resid 404 and name CA)	14.62	0.27	0.26
55	assign (segid 3A4 and resid 258 and name CA) (segid 3A4 and resid 404 and name CB)	13.21	0.27	0.27
	assign (segid 3A4 and resid 258 and name CA) (segid 3A4 and resid 405 and name CA)	15.67	0.58	0.57
	assign (segid 3A4 and resid 258 and name CA) (segid 3A4 and resid 405 and name CB)	15.18	0.63	0.62
	assign (segid 3A4 and resid 258 and name CA) (segid 3A4 and resid 406 and name CA)	18.95	0.54	0.53
	assign (segid 3A4 and resid 258 and name CA) (segid 3A4 and resid 407 and name CB)	19.34	0.30	0.31
60	assign (segid 3A4 and resid 258 and name CA) (segid 3A4 and resid 408 and name CA)	18.93	0.31	0.30
	assign (segid 3A4 and resid 258 and name CA) (segid 3A4 and resid 408 and name CB)	17.68	0.31	0.31
	assign (segid 3A4 and resid 258 and name CA) (segid 3A4 and resid 425 and name CA)	16.98	0.88	0.88
	assign (segid 3A4 and resid 258 and name CA) (segid 3A4 and resid 426 and name CA)	14.77	1.37	1.36
65	assign (segid 3A4 and resid 258 and name CA) (segid 3A4 and resid 427 and name CA)	13.10	0.92	0.91
	assign (segid 3A4 and resid 258 and name CA) (segid 3A4 and resid 428 and name CA)	13.80	0.74	0.74
	assign (segid 3A4 and resid 258 and name CA) (segid 3A4 and resid 429 and name CA)	12.96	1.10	1.10
	assign (segid 3A4 and resid 258 and name CA) (segid 3A4 and resid 430 and name CA)	12.84	1.27	1.28
	assign (segid 3A4 and resid 258 and name CA) (segid 3A4 and resid 431 and name CA)	10.41	0.73	0.72
70	assign (segid 3A4 and resid 258 and name CA) (segid 3A4 and resid 433 and name CA)	8.58	0.55	0.55
	assign (segid 3A4 and resid 258 and name CA) (segid 3A4 and resid 434 and name CA)	8.52	0.47	0.47
	assign (segid 3A4 and resid 258 and name CA) (segid 3A4 and resid 435 and name CA)	11.11	0.66	0.67
	assign (segid 3A4 and resid 258 and name CA) (segid 3A4 and resid 436 and name CA)	13.02	1.28	1.29
	assign (segid 3A4 and resid 258 and name CA) (segid 3A4 and resid 437 and name CA)	15.36	0.90	0.90
	assign (segid 3A4 and resid 258 and name CA) (segid 3A4 and resid 438 and name CA)	16.23	0.77	0.77
75	assign (segid 3A4 and resid 258 and name CA) (segid 3A4 and resid 439 and name CA)	19.37	0.44	0.44
	assign (segid 3A4 and resid 258 and name CA) (segid HEM and resid 1 and name C1B)	5.91	0.27	0.27
	assign (segid 3A4 and resid 258 and name CA) (segid HEM and resid 1 and name C1C)	6.42	0.31	0.30
	assign (segid 3A4 and resid 258 and name CA) (segid HEM and resid 1 and name C2B)	5.26	0.26	0.27
	assign (segid 3A4 and resid 258 and name CA) (segid HEM and resid 1 and name C2C)	7.05	0.32	0.32
80	assign (segid 3A4 and resid 258 and name CA) (segid HEM and resid 1 and name C3B)	4.83	0.23	0.24
	assign (segid 3A4 and resid 258 and name CA) (segid HEM and resid 1 and name C4B)	5.28	0.26	0.26
	assign (segid 3A4 and resid 258 and name CA) (segid HEM and resid 1 and name CAB)	4.62	0.20	0.20
	assign (segid 3A4 and resid 258 and name CA) (segid HEM and resid 1 and name CBB)	4.88	0.31	0.31

	assign (segid 3A4 and resid 258 and name CA) (segid HEM and resid 1 and name CHB)	6.81	0.25	0.26
	assign (segid 3A4 and resid 258 and name CA) (segid HEM and resid 1 and name CHC)	5.54	0.27	0.28
	assign (segid 3A4 and resid 258 and name CA) (segid HEM and resid 1 and name CMB)	5.63	0.35	0.34
	assign (segid 3A4 and resid 258 and name CA) (segid HEM and resid 1 and name CMC)	7.08	0.34	0.33
5	assign (segid 3A4 and resid 258 and name CA) (segid HEM and resid 1 and name NB)	5.93	0.28	0.29
	assign (segid 3A4 and resid 258 and name CA) (segid HEM and resid 1 and name NC)	7.09	0.30	0.31
	assign (segid 3A4 and resid 258 and name CB) (segid 3A4 and resid 259 and name C)	5.45	0.08	0.08
	assign (segid 3A4 and resid 258 and name CB) (segid 3A4 and resid 259 and name CA)	4.46	0.09	0.08
	assign (segid 3A4 and resid 258 and name CB) (segid 3A4 and resid 259 and name CB)	5.25	0.12	0.12
10	assign (segid 3A4 and resid 258 and name CB) (segid 3A4 and resid 259 and name N)	3.12	0.10	0.10
	assign (segid 3A4 and resid 258 and name CB) (segid 3A4 and resid 259 and name O)	6.36	0.07	0.07
	assign (segid 3A4 and resid 258 and name CB) (segid 3A4 and resid 260 and name C)	7.01	0.09	0.09
	assign (segid 3A4 and resid 258 and name CB) (segid 3A4 and resid 260 and name CA)	6.85	0.12	0.13
	assign (segid 3A4 and resid 258 and name CB) (segid 3A4 and resid 260 and name CB)	7.27	0.25	0.25
15	assign (segid 3A4 and resid 258 and name CB) (segid 3A4 and resid 260 and name N)	5.63	0.12	0.12
	assign (segid 3A4 and resid 258 and name CB) (segid 3A4 and resid 261 and name C)	7.05	0.19	0.19
	assign (segid 3A4 and resid 258 and name CB) (segid 3A4 and resid 261 and name CA)	6.70	0.21	0.20
	assign (segid 3A4 and resid 258 and name CB) (segid 3A4 and resid 261 and name N)	6.17	0.12	0.12
	assign (segid 3A4 and resid 258 and name CB) (segid 3A4 and resid 262 and name CA)	7.10	0.15	0.15
20	assign (segid 3A4 and resid 258 and name CB) (segid 3A4 and resid 262 and name CB)	6.48	0.13	0.14
	assign (segid 3A4 and resid 258 and name CB) (segid 3A4 and resid 262 and name N)	6.36	0.17	0.18
	assign (segid 3A4 and resid 258 and name CB) (segid 3A4 and resid 263 and name CA)	9.84	0.11	0.11
	assign (segid 3A4 and resid 258 and name CB) (segid 3A4 and resid 263 and name CB)	9.97	0.11	0.10
	assign (segid 3A4 and resid 258 and name CB) (segid 3A4 and resid 264 and name CA)	11.41	0.18	0.17
25	assign (segid 3A4 and resid 258 and name CB) (segid 3A4 and resid 265 and name CA)	11.59	0.39	0.38
	assign (segid 3A4 and resid 258 and name CB) (segid 3A4 and resid 266 and name CA)	13.02	0.30	0.31
	assign (segid 3A4 and resid 258 and name CB) (segid 3A4 and resid 267 and name CA)	15.55	0.20	0.20
	assign (segid 3A4 and resid 258 and name CB) (segid 3A4 and resid 267 and name CB)	15.44	0.19	0.20
	assign (segid 3A4 and resid 258 and name CB) (segid 3A4 and resid 268 and name CA)	16.59	0.29	0.29
30	assign (segid 3A4 and resid 258 and name CB) (segid 3A4 and resid 268 and name CB)	15.89	0.34	0.35
	assign (segid 3A4 and resid 258 and name CB) (segid 3A4 and resid 269 and name CA)	17.30	0.49	0.48
	assign (segid 3A4 and resid 258 and name CB) (segid 3A4 and resid 270 and name CA)	19.24	0.27	0.27
	assign (segid 3A4 and resid 258 and name CB) (segid 3A4 and resid 270 and name CB)	18.88	0.24	0.23
	assign (segid 3A4 and resid 258 and name CB) (segid 3A4 and resid 306 and name CA)	17.43	0.68	0.67
35	assign (segid 3A4 and resid 258 and name CB) (segid 3A4 and resid 307 and name CA)	18.46	0.71	0.72
	assign (segid 3A4 and resid 258 and name CB) (segid 3A4 and resid 308 and name CA)	17.09	0.65	0.64
	assign (segid 3A4 and resid 258 and name CB) (segid 3A4 and resid 308 and name CB)	17.57	0.64	0.64
	assign (segid 3A4 and resid 258 and name CB) (segid 3A4 and resid 309 and name CA)	13.56	0.67	0.66
	assign (segid 3A4 and resid 258 and name CB) (segid 3A4 and resid 309 and name CB)	13.31	0.71	0.70
40	assign (segid 3A4 and resid 258 and name CB) (segid 3A4 and resid 310 and name CA)	14.02	0.69	0.70
	assign (segid 3A4 and resid 258 and name CB) (segid 3A4 and resid 310 and name CB)	15.22	0.72	0.73
	assign (segid 3A4 and resid 258 and name CB) (segid 3A4 and resid 311 and name CA)	15.45	0.65	0.66
	assign (segid 3A4 and resid 258 and name CB) (segid 3A4 and resid 311 and name CB)	16.79	0.67	0.68
45	assign (segid 3A4 and resid 258 and name CB) (segid 3A4 and resid 312 and name CA)	12.80	0.68	0.67
	assign (segid 3A4 and resid 258 and name CB) (segid 3A4 and resid 312 and name CB)	12.41	0.71	0.71
	assign (segid 3A4 and resid 258 and name CB) (segid 3A4 and resid 313 and name CA)	10.20	0.64	0.63
	assign (segid 3A4 and resid 258 and name CB) (segid 3A4 and resid 313 and name CB)	9.89	0.67	0.67
	assign (segid 3A4 and resid 258 and name CB) (segid 3A4 and resid 314 and name CA)	13.17	0.59	0.59
	assign (segid 3A4 and resid 258 and name CB) (segid 3A4 and resid 314 and name CB)	14.57	0.60	0.60
50	assign (segid 3A4 and resid 258 and name CB) (segid 3A4 and resid 315 and name CA)	14.24	0.53	0.54
	assign (segid 3A4 and resid 258 and name CB) (segid 3A4 and resid 315 and name CB)	15.01	0.63	0.62
	assign (segid 3A4 and resid 258 and name CB) (segid 3A4 and resid 316 and name CA)	11.26	0.59	0.60
	assign (segid 3A4 and resid 258 and name CB) (segid 3A4 and resid 317 and name CA)	9.40	0.73	0.73
	assign (segid 3A4 and resid 258 and name CB) (segid 3A4 and resid 318 and name CA)	6.62	0.91	0.91
55	assign (segid 3A4 and resid 258 and name CB) (segid 3A4 and resid 318 and name CB)	5.52	0.94	0.95
	assign (segid 3A4 and resid 258 and name CB) (segid 3A4 and resid 319 and name CA)	6.95	0.90	0.89
	assign (segid 3A4 and resid 258 and name CB) (segid 3A4 and resid 319 and name CB)	6.40	0.83	0.83
	assign (segid 3A4 and resid 258 and name CB) (segid 3A4 and resid 322 and name CA)	16.03	0.42	0.42
	assign (segid 3A4 and resid 258 and name CB) (segid 3A4 and resid 323 and name CA)	18.88	0.66	0.65
60	assign (segid 3A4 and resid 258 and name CB) (segid 3A4 and resid 344 and name CA)	17.91	0.18	0.19
	assign (segid 3A4 and resid 258 and name CB) (segid 3A4 and resid 344 and name CB)	17.93	0.24	0.23
	assign (segid 3A4 and resid 258 and name CB) (segid 3A4 and resid 345 and name CA)	16.63	0.41	0.41
	assign (segid 3A4 and resid 258 and name CB) (segid 3A4 and resid 345 and name CB)	16.39	0.65	0.64
	assign (segid 3A4 and resid 258 and name CB) (segid 3A4 and resid 346 and name CA)	15.37	0.55	0.54
65	assign (segid 3A4 and resid 258 and name CB) (segid 3A4 and resid 346 and name CB)	16.38	0.67	0.67
	assign (segid 3A4 and resid 258 and name CB) (segid 3A4 and resid 347 and name CA)	13.21	0.53	0.53
	assign (segid 3A4 and resid 258 and name CB) (segid 3A4 and resid 347 and name CB)	11.83	0.54	0.55
	assign (segid 3A4 and resid 258 and name CB) (segid 3A4 and resid 348 and name CA)	13.52	0.66	0.66
	assign (segid 3A4 and resid 258 and name CB) (segid 3A4 and resid 349 and name CA)	17.22	0.56	0.57
70	assign (segid 3A4 and resid 258 and name CB) (segid 3A4 and resid 349 and name CB)	18.02	0.53	0.53
	assign (segid 3A4 and resid 258 and name CB) (segid 3A4 and resid 350 and name CA)	17.49	0.31	0.32
	assign (segid 3A4 and resid 258 and name CB) (segid 3A4 and resid 350 and name CB)	16.89	0.35	0.34
	assign (segid 3A4 and resid 258 and name CB) (segid 3A4 and resid 351 and name CA)	16.20	0.51	0.51
	assign (segid 3A4 and resid 258 and name CB) (segid 3A4 and resid 352 and name CA)	18.78	0.35	0.35
75	assign (segid 3A4 and resid 258 and name CB) (segid 3A4 and resid 352 and name CB)	18.54	0.39	0.39
	assign (segid 3A4 and resid 258 and name CB) (segid 3A4 and resid 381 and name CA)	15.32	0.38	0.38
	assign (segid 3A4 and resid 258 and name CB) (segid 3A4 and resid 382 and name CA)	13.22	0.27	0.28
	assign (segid 3A4 and resid 258 and name CB) (segid 3A4 and resid 382 and name CB)	14.02	0.30	0.29
	assign (segid 3A4 and resid 258 and name CB) (segid 3A4 and resid 383 and name CA)	9.67	0.33	0.32
80	assign (segid 3A4 and resid 258 and name CB) (segid 3A4 and resid 384 and name CA)	9.03	0.23	0.24
	assign (segid 3A4 and resid 258 and name CB) (segid 3A4 and resid 384 and name CB)	9.46	0.22	0.22
	assign (segid 3A4 and resid 258 and name CB) (segid 3A4 and resid 385 and name CA)	11.61	0.22	0.22
	assign (segid 3A4 and resid 258 and name CB) (segid 3A4 and resid 386 and name CA)	15.16	0.22	0.22

	assign (segid 3A4 and resid 258 and name CB)	(segid 3A4 and resid 387 and name CA)	17.59	0.42	0.42
	assign (segid 3A4 and resid 258 and name CB)	(segid 3A4 and resid 388 and name CA)	17.90	0.28	0.28
	assign (segid 3A4 and resid 258 and name CB)	(segid 3A4 and resid 388 and name CB)	19.04	0.31	0.31
	assign (segid 3A4 and resid 258 and name CB)	(segid 3A4 and resid 389 and name CA)	14.60	0.33	0.33
5	assign (segid 3A4 and resid 258 and name CB)	(segid 3A4 and resid 389 and name CB)	14.54	0.47	0.47
	assign (segid 3A4 and resid 258 and name CB)	(segid 3A4 and resid 390 and name CA)	12.78	0.32	0.32
	assign (segid 3A4 and resid 258 and name CB)	(segid 3A4 and resid 390 and name CB)	13.68	0.39	0.39
	assign (segid 3A4 and resid 258 and name CB)	(segid 3A4 and resid 391 and name CA)	9.69	0.35	0.35
	assign (segid 3A4 and resid 258 and name CB)	(segid 3A4 and resid 391 and name CB)	8.52	0.34	0.34
10	assign (segid 3A4 and resid 258 and name CB)	(segid 3A4 and resid 392 and name CA)	11.52	0.43	0.44
	assign (segid 3A4 and resid 258 and name CB)	(segid 3A4 and resid 392 and name CB)	12.03	0.46	0.46
	assign (segid 3A4 and resid 258 and name CB)	(segid 3A4 and resid 393 and name CA)	9.35	0.57	0.57
	assign (segid 3A4 and resid 258 and name CB)	(segid 3A4 and resid 394 and name CA)	9.66	0.44	0.44
	assign (segid 3A4 and resid 258 and name CB)	(segid 3A4 and resid 394 and name CB)	10.51	0.45	0.46
15	assign (segid 3A4 and resid 258 and name CB)	(segid 3A4 and resid 395 and name CA)	12.51	0.44	0.43
	assign (segid 3A4 and resid 258 and name CB)	(segid 3A4 and resid 396 and name CA)	11.21	0.55	0.54
	assign (segid 3A4 and resid 258 and name CB)	(segid 3A4 and resid 396 and name CB)	10.98	0.64	0.64
	assign (segid 3A4 and resid 258 and name CB)	(segid 3A4 and resid 397 and name CA)	8.21	0.37	0.38
	assign (segid 3A4 and resid 258 and name CB)	(segid 3A4 and resid 397 and name CB)	7.15	0.35	0.35
20	assign (segid 3A4 and resid 258 and name CB)	(segid 3A4 and resid 398 and name CA)	11.04	0.27	0.26
	assign (segid 3A4 and resid 258 and name CB)	(segid 3A4 and resid 398 and name CB)	11.89	0.27	0.27
	assign (segid 3A4 and resid 258 and name CB)	(segid 3A4 and resid 399 and name CA)	13.43	0.36	0.36
	assign (segid 3A4 and resid 258 and name CB)	(segid 3A4 and resid 399 and name CB)	13.97	0.39	0.38
	assign (segid 3A4 and resid 258 and name CB)	(segid 3A4 and resid 400 and name CA)	11.76	0.45	0.44
25	assign (segid 3A4 and resid 258 and name CB)	(segid 3A4 and resid 400 and name CB)	10.59	0.53	0.53
	assign (segid 3A4 and resid 258 and name CB)	(segid 3A4 and resid 401 and name CA)	11.28	0.24	0.25
	assign (segid 3A4 and resid 258 and name CB)	(segid 3A4 and resid 402 and name CA)	14.83	0.24	0.23
	assign (segid 3A4 and resid 258 and name CB)	(segid 3A4 and resid 402 and name CB)	15.38	0.24	0.24
	assign (segid 3A4 and resid 258 and name CB)	(segid 3A4 and resid 403 and name CA)	16.35	0.25	0.24
30	assign (segid 3A4 and resid 258 and name CB)	(segid 3A4 and resid 403 and name CB)	16.21	0.25	0.25
	assign (segid 3A4 and resid 258 and name CB)	(segid 3A4 and resid 404 and name CA)	15.19	0.27	0.27
	assign (segid 3A4 and resid 258 and name CB)	(segid 3A4 and resid 404 and name CB)	13.84	0.27	0.27
	assign (segid 3A4 and resid 258 and name CB)	(segid 3A4 and resid 405 and name CA)	16.26	0.54	0.53
	assign (segid 3A4 and resid 258 and name CB)	(segid 3A4 and resid 405 and name CB)	15.70	0.58	0.58
35	assign (segid 3A4 and resid 258 and name CB)	(segid 3A4 and resid 408 and name CB)	18.57	0.28	0.28
	assign (segid 3A4 and resid 258 and name CB)	(segid 3A4 and resid 426 and name CA)	15.88	1.46	1.47
	assign (segid 3A4 and resid 258 and name CB)	(segid 3A4 and resid 427 and name CA)	14.14	0.95	0.95
	assign (segid 3A4 and resid 258 and name CB)	(segid 3A4 and resid 428 and name CA)	14.65	0.66	0.67
	assign (segid 3A4 and resid 258 and name CB)	(segid 3A4 and resid 429 and name CA)	13.57	1.05	1.05
40	assign (segid 3A4 and resid 258 and name CB)	(segid 3A4 and resid 430 and name CA)	13.14	1.19	1.18
	assign (segid 3A4 and resid 258 and name CB)	(segid 3A4 and resid 431 and name CA)	10.42	0.78	0.78
	assign (segid 3A4 and resid 258 and name CB)	(segid 3A4 and resid 433 and name CA)	9.27	0.48	0.48
	assign (segid 3A4 and resid 258 and name CB)	(segid 3A4 and resid 434 and name CA)	9.67	0.51	0.51
	assign (segid 3A4 and resid 258 and name CB)	(segid 3A4 and resid 435 and name CA)	12.44	0.66	0.66
45	assign (segid 3A4 and resid 258 and name CB)	(segid 3A4 and resid 436 and name CA)	14.44	1.25	1.26
	assign (segid 3A4 and resid 258 and name CB)	(segid 3A4 and resid 437 and name CA)	16.85	0.89	0.89
	assign (segid 3A4 and resid 258 and name CB)	(segid 3A4 and resid 438 and name CA)	17.69	0.75	0.74
	assign (segid 3A4 and resid 258 and name CB)	(segid HEM and resid 1 and name C1B)	4.49	0.24	0.24
	assign (segid 3A4 and resid 258 and name CB)	(segid HEM and resid 1 and name C1C)	5.19	0.41	0.41
50	assign (segid 3A4 and resid 258 and name CB)	(segid HEM and resid 1 and name C2B)	4.04	0.22	0.22
	assign (segid 3A4 and resid 258 and name CB)	(segid HEM and resid 1 and name C2C)	6.02	0.44	0.43
	assign (segid 3A4 and resid 258 and name CB)	(segid HEM and resid 1 and name C3A)	7.41	0.28	0.28
	assign (segid 3A4 and resid 258 and name CB)	(segid HEM and resid 1 and name C3B)	3.66	0.19	0.20
	assign (segid 3A4 and resid 258 and name CB)	(segid HEM and resid 1 and name C3C)	6.89	0.44	0.43
55	assign (segid 3A4 and resid 258 and name CB)	(segid HEM and resid 1 and name C4A)	6.29	0.25	0.25
	assign (segid 3A4 and resid 258 and name CB)	(segid HEM and resid 1 and name C4B)	3.93	0.29	0.29
	assign (segid 3A4 and resid 258 and name CB)	(segid HEM and resid 1 and name C4C)	6.71	0.41	0.41
	assign (segid 3A4 and resid 258 and name CB)	(segid HEM and resid 1 and name CAB)	3.82	0.14	0.14
	assign (segid 3A4 and resid 258 and name CB)	(segid HEM and resid 1 and name CBB)	4.42	0.27	0.27
60	assign (segid 3A4 and resid 258 and name CB)	(segid HEM and resid 1 and name CHB)	5.41	0.23	0.23
	assign (segid 3A4 and resid 258 and name CB)	(segid HEM and resid 1 and name CHC)	4.33	0.36	0.37
	assign (segid 3A4 and resid 258 and name CB)	(segid HEM and resid 1 and name CHB)	4.66	0.30	0.29
	assign (segid 3A4 and resid 258 and name CB)	(segid HEM and resid 1 and name CMC)	6.30	0.45	0.45
	assign (segid 3A4 and resid 258 and name CB)	(segid HEM and resid 1 and name FE)	5.87	0.36	0.35
65	assign (segid 3A4 and resid 258 and name CB)	(segid HEM and resid 1 and name NA)	6.52	0.29	0.29
	assign (segid 3A4 and resid 258 and name CB)	(segid HEM and resid 1 and name NB)	4.46	0.29	0.29
	assign (segid 3A4 and resid 258 and name CB)	(segid HEM and resid 1 and name NC)	5.74	0.38	0.38
	assign (segid 3A4 and resid 258 and name N)	(segid 3A4 and resid 258 and name C)	2.47	0.02	0.03
	assign (segid 3A4 and resid 258 and name N)	(segid 3A4 and resid 258 and name CA)	1.46	0.01	0.00
70	assign (segid 3A4 and resid 258 and name N)	(segid 3A4 and resid 258 and name CB)	2.46	0.05	0.04
	assign (segid 3A4 and resid 258 and name N)	(segid 3A4 and resid 258 and name O)	3.46	0.07	0.06
	assign (segid 3A4 and resid 258 and name N)	(segid 3A4 and resid 259 and name C)	4.77	0.04	0.04
	assign (segid 3A4 and resid 258 and name N)	(segid 3A4 and resid 259 and name CA)	4.29	0.07	0.07
	assign (segid 3A4 and resid 258 and name N)	(segid 3A4 and resid 259 and name CB)	5.08	0.10	0.11
75	assign (segid 3A4 and resid 258 and name N)	(segid 3A4 and resid 259 and name N)	2.89	0.08	0.08
	assign (segid 3A4 and resid 258 and name N)	(segid 3A4 and resid 259 and name O)	5.85	0.04	0.05
	assign (segid 3A4 and resid 258 and name N)	(segid 3A4 and resid 260 and name C)	5.69	0.03	0.02
	assign (segid 3A4 and resid 258 and name N)	(segid 3A4 and resid 260 and name CA)	5.36	0.12	0.12
	assign (segid 3A4 and resid 258 and name N)	(segid 3A4 and resid 260 and name CB)	5.36	0.29	0.29
80	assign (segid 3A4 and resid 258 and name N)	(segid 3A4 and resid 260 and name N)	4.36	0.07	0.08
	assign (segid 3A4 and resid 258 and name N)	(segid 3A4 and resid 260 and name O)	6.89	0.02	0.02
	assign (segid 3A4 and resid 258 and name N)	(segid 3A4 and resid 261 and name C)	6.49	0.13	0.13
	assign (segid 3A4 and resid 258 and name N)	(segid 3A4 and resid 261 and name CA)	5.68	0.13	0.14

	assign (segid 3A4 and resid 258 and name N)	(segid 3A4 and resid 261 and name N)	4.89	0.05	0.05
	assign (segid 3A4 and resid 258 and name N)	(segid 3A4 and resid 261 and name O)	7.68	0.15	0.15
	assign (segid 3A4 and resid 258 and name N)	(segid 3A4 and resid 262 and name CA)	7.25	0.09	0.10
	assign (segid 3A4 and resid 258 and name N)	(segid 3A4 and resid 262 and name CB)	7.04	0.07	0.06
5	assign (segid 3A4 and resid 258 and name N)	(segid 3A4 and resid 262 and name N)	6.14	0.10	0.11
	assign (segid 3A4 and resid 258 and name N)	(segid HEM and resid 1 and name C1B)	6.87	0.24	0.24
	assign (segid 3A4 and resid 258 and name N)	(segid HEM and resid 1 and name C1C)	6.73	0.22	0.23
	assign (segid 3A4 and resid 258 and name N)	(segid HEM and resid 1 and name C2B)	6.43	0.25	0.24
	assign (segid 3A4 and resid 258 and name N)	(segid HEM and resid 1 and name C2C)	7.16	0.26	0.26
10	assign (segid 3A4 and resid 258 and name N)	(segid HEM and resid 1 and name C3B)	5.91	0.19	0.20
	assign (segid 3A4 and resid 258 and name N)	(segid HEM and resid 1 and name C4B)	6.08	0.19	0.20
	assign (segid 3A4 and resid 258 and name N)	(segid HEM and resid 1 and name C4B)	5.75	0.19	0.18
	assign (segid 3A4 and resid 258 and name N)	(segid HEM and resid 1 and name CBB)	6.13	0.27	0.28
	assign (segid 3A4 and resid 258 and name N)	(segid HEM and resid 1 and name CHC)	6.11	0.19	0.20
15	assign (segid 3A4 and resid 258 and name N)	(segid HEM and resid 1 and name CMB)	6.94	0.32	0.33
	assign (segid 3A4 and resid 258 and name N)	(segid HEM and resid 1 and name CMC)	7.16	0.28	0.29
	assign (segid 3A4 and resid 258 and name N)	(segid HEM and resid 1 and name NB)	6.70	0.23	0.22
	assign (segid 3A4 and resid 258 and name N)	(segid HEM and resid 1 and name NC)	7.37	0.24	0.24
	assign (segid 3A4 and resid 258 and name N)	(segid 3A4 and resid 258 and name CB)	3.39	0.08	0.09
20	assign (segid 3A4 and resid 258 and name O)	(segid 3A4 and resid 259 and name C)	3.00	0.07	0.07
	assign (segid 3A4 and resid 258 and name O)	(segid 3A4 and resid 259 and name CA)	2.76	0.05	0.05
	assign (segid 3A4 and resid 258 and name O)	(segid 3A4 and resid 259 and name CB)	4.23	0.05	0.06
	assign (segid 3A4 and resid 258 and name O)	(segid 3A4 and resid 259 and name N)	2.24	0.01	0.02
	assign (segid 3A4 and resid 258 and name O)	(segid 3A4 and resid 259 and name O)	3.51	0.09	0.08
25	assign (segid 3A4 and resid 258 and name O)	(segid 3A4 and resid 260 and name C)	4.13	0.13	0.12
	assign (segid 3A4 and resid 258 and name O)	(segid 3A4 and resid 260 and name CA)	4.39	0.16	0.16
	assign (segid 3A4 and resid 258 and name O)	(segid 3A4 and resid 260 and name CB)	5.29	0.26	0.27
	assign (segid 3A4 and resid 258 and name O)	(segid 3A4 and resid 260 and name N)	3.44	0.14	0.13
	assign (segid 3A4 and resid 258 and name O)	(segid 3A4 and resid 260 and name O)	5.03	0.11	0.11
30	assign (segid 3A4 and resid 258 and name O)	(segid 3A4 and resid 261 and name C)	3.86	0.07	0.08
	assign (segid 3A4 and resid 258 and name O)	(segid 3A4 and resid 261 and name CA)	3.83	0.10	0.10
	assign (segid 3A4 and resid 258 and name O)	(segid 3A4 and resid 261 and name N)	3.36	0.13	0.13
	assign (segid 3A4 and resid 258 and name O)	(segid 3A4 and resid 261 and name O)	5.03	0.09	0.09
	assign (segid 3A4 and resid 258 and name O)	(segid 3A4 and resid 262 and name C)	5.11	0.09	0.10
35	assign (segid 3A4 and resid 258 and name O)	(segid 3A4 and resid 262 and name CA)	3.91	0.09	0.09
	assign (segid 3A4 and resid 258 and name O)	(segid 3A4 and resid 262 and name CB)	3.62	0.11	0.11
	assign (segid 3A4 and resid 258 and name O)	(segid 3A4 and resid 262 and name N)	3.06	0.10	0.09
	assign (segid 3A4 and resid 258 and name O)	(segid 3A4 and resid 262 and name O)	6.22	0.10	0.10
40	assign (segid 3A4 and resid 258 and name O)	(segid 3A4 and resid 263 and name C)	7.39	0.08	0.08
	assign (segid 3A4 and resid 258 and name O)	(segid 3A4 and resid 263 and name CA)	6.57	0.10	0.10
	assign (segid 3A4 and resid 258 and name O)	(segid 3A4 and resid 263 and name CB)	6.84	0.11	0.11
	assign (segid 3A4 and resid 258 and name O)	(segid 3A4 and resid 263 and name CG)	6.67	0.27	0.28
	assign (segid 3A4 and resid 258 and name O)	(segid 3A4 and resid 263 and name N)	5.18	0.09	0.10
	assign (segid 3A4 and resid 258 and name O)	(segid 3A4 and resid 264 and name N)	7.04	0.08	0.08
45	assign (segid 3A4 and resid 258 and name O)	(segid 3A4 and resid 318 and name C)	6.89	0.64	0.65
	assign (segid 3A4 and resid 258 and name O)	(segid 3A4 and resid 318 and name CA)	6.31	0.72	0.71
	assign (segid 3A4 and resid 258 and name O)	(segid 3A4 and resid 318 and name CB)	4.88	0.77	0.76
	assign (segid 3A4 and resid 258 and name O)	(segid 3A4 and resid 318 and name O)	7.15	0.60	0.60
	assign (segid 3A4 and resid 258 and name O)	(segid 3A4 and resid 433 and name O)	6.52	0.45	0.45
50	assign (segid 3A4 and resid 258 and name O)	(segid HEM and resid 1 and name C1B)	6.79	0.24	0.24
	assign (segid 3A4 and resid 258 and name O)	(segid HEM and resid 1 and name C1C)	7.52	0.19	0.18
	assign (segid 3A4 and resid 258 and name O)	(segid HEM and resid 1 and name C2B)	5.70	0.27	0.27
	assign (segid 3A4 and resid 258 and name O)	(segid HEM and resid 1 and name C3B)	5.19	0.25	0.25
	assign (segid 3A4 and resid 258 and name O)	(segid HEM and resid 1 and name C4B)	6.09	0.22	0.23
55	assign (segid 3A4 and resid 258 and name O)	(segid HEM and resid 1 and name C4B)	4.41	0.26	0.26
	assign (segid 3A4 and resid 258 and name O)	(segid HEM and resid 1 and name CBB)	4.00	0.38	0.37
	assign (segid 3A4 and resid 258 and name O)	(segid HEM and resid 1 and name CHC)	6.39	0.19	0.18
	assign (segid 3A4 and resid 258 and name O)	(segid HEM and resid 1 and name CMB)	5.67	0.35	0.35
	assign (segid 3A4 and resid 258 and name O)	(segid HEM and resid 1 and name NB)	7.00	0.23	0.23
60	assign (segid 3A4 and resid 258 and name O)	(segid 3A4 and resid 259 and name CB)	2.51	0.04	0.04
	assign (segid 3A4 and resid 259 and name C)	(segid 3A4 and resid 259 and name O)	1.23	0.01	0.01
	assign (segid 3A4 and resid 259 and name C)	(segid 3A4 and resid 260 and name C)	3.01	0.05	0.04
	assign (segid 3A4 and resid 259 and name C)	(segid 3A4 and resid 260 and name CA)	2.44	0.03	0.02
	assign (segid 3A4 and resid 259 and name C)	(segid 3A4 and resid 260 and name CB)	3.72	0.04	0.04
65	assign (segid 3A4 and resid 259 and name C)	(segid 3A4 and resid 260 and name N)	1.33	0.02	0.02
	assign (segid 3A4 and resid 259 and name C)	(segid 3A4 and resid 260 and name O)	3.81	0.06	0.06
	assign (segid 3A4 and resid 259 and name C)	(segid 3A4 and resid 261 and name C)	4.54	0.08	0.09
	assign (segid 3A4 and resid 259 and name C)	(segid 3A4 and resid 261 and name CA)	4.49	0.07	0.08
	assign (segid 3A4 and resid 259 and name C)	(segid 3A4 and resid 261 and name N)	3.33	0.06	0.07
70	assign (segid 3A4 and resid 259 and name C)	(segid 3A4 and resid 261 and name O)	5.60	0.12	0.13
	assign (segid 3A4 and resid 259 and name C)	(segid 3A4 and resid 262 and name C)	4.91	0.03	0.03
	assign (segid 3A4 and resid 259 and name C)	(segid 3A4 and resid 262 and name CA)	4.53	0.07	0.06
	assign (segid 3A4 and resid 259 and name C)	(segid 3A4 and resid 262 and name CB)	4.29	0.11	0.11
	assign (segid 3A4 and resid 259 and name C)	(segid 3A4 and resid 262 and name N)	3.81	0.08	0.09
75	assign (segid 3A4 and resid 259 and name C)	(segid 3A4 and resid 262 and name O)	6.12	0.03	0.04
	assign (segid 3A4 and resid 259 and name C)	(segid 3A4 and resid 263 and name C)	6.23	0.05	0.05
	assign (segid 3A4 and resid 259 and name C)	(segid 3A4 and resid 263 and name CA)	5.17	0.06	0.06
	assign (segid 3A4 and resid 259 and name C)	(segid 3A4 and resid 263 and name CB)	4.80	0.07	0.08
	assign (segid 3A4 and resid 259 and name C)	(segid 3A4 and resid 263 and name CG)	4.39	0.23	0.24
80	assign (segid 3A4 and resid 259 and name C)	(segid 3A4 and resid 263 and name N)	4.21	0.04	0.04
	assign (segid 3A4 and resid 259 and name C)	(segid 3A4 and resid 263 and name O)	7.40	0.06	0.06
	assign (segid 3A4 and resid 259 and name C)	(segid 3A4 and resid 264 and name CA)	7.34	0.11	0.11
	assign (segid 3A4 and resid 259 and name C)	(segid 3A4 and resid 264 and name N)	6.07	0.09	0.08

	assign (segid 3A4 and resid 259 and name C) (segid 3A4 and resid 397 and name O)	7.32	0.31	0.31
	assign (segid 3A4 and resid 259 and name C) (segid HEM and resid 1 and name C3B)	6.84	0.17	0.17
	assign (segid 3A4 and resid 259 and name C) (segid HEM and resid 1 and name C4B)	7.49	0.19	0.20
	assign (segid 3A4 and resid 259 and name C) (segid HEM and resid 1 and name CAB)	5.71	0.16	0.16
5	assign (segid 3A4 and resid 259 and name C) (segid HEM and resid 1 and name CBB)	5.33	0.25	0.26
	assign (segid 3A4 and resid 259 and name C) (segid HEM and resid 1 and name CHC)	7.25	0.17	0.17
	assign (segid 3A4 and resid 259 and name C) (segid HEM and resid 1 and name CMC)	7.46	0.18	0.18
	assign (segid 3A4 and resid 259 and name CA) (segid 3A4 and resid 259 and name C)	1.52	0.01	0.01
	assign (segid 3A4 and resid 259 and name CA) (segid 3A4 and resid 259 and name CB)	1.52	0.00	0.01
10	assign (segid 3A4 and resid 259 and name CA) (segid 3A4 and resid 259 and name O)	2.39	0.02	0.02
	assign (segid 3A4 and resid 259 and name CA) (segid 3A4 and resid 260 and name C)	4.40	0.03	0.04
	assign (segid 3A4 and resid 259 and name CA) (segid 3A4 and resid 260 and name CA)	3.82	0.01	0.02
	assign (segid 3A4 and resid 259 and name CA) (segid 3A4 and resid 260 and name CB)	4.88	0.04	0.05
	assign (segid 3A4 and resid 259 and name CA) (segid 3A4 and resid 260 and name N)	2.45	0.03	0.02
15	assign (segid 3A4 and resid 259 and name CA) (segid 3A4 and resid 260 and name O)	5.27	0.05	0.05
	assign (segid 3A4 and resid 259 and name CA) (segid 3A4 and resid 261 and name C)	5.46	0.10	0.10
	assign (segid 3A4 and resid 259 and name CA) (segid 3A4 and resid 261 and name CA)	5.48	0.10	0.09
	assign (segid 3A4 and resid 259 and name CA) (segid 3A4 and resid 261 and name N)	4.43	0.08	0.07
	assign (segid 3A4 and resid 259 and name CA) (segid 3A4 and resid 261 and name O)	6.57	0.11	0.12
20	assign (segid 3A4 and resid 259 and name CA) (segid 3A4 and resid 262 and name C)	5.70	0.06	0.06
	assign (segid 3A4 and resid 259 and name CA) (segid 3A4 and resid 262 and name CA)	5.07	0.09	0.09
	assign (segid 3A4 and resid 259 and name CA) (segid 3A4 and resid 262 and name CB)	4.41	0.11	0.11
	assign (segid 3A4 and resid 259 and name CA) (segid 3A4 and resid 262 and name N)	4.53	0.10	0.10
	assign (segid 3A4 and resid 259 and name CA) (segid 3A4 and resid 262 and name O)	6.87	0.07	0.07
25	assign (segid 3A4 and resid 259 and name CA) (segid 3A4 and resid 263 and name C)	7.45	0.08	0.07
	assign (segid 3A4 and resid 259 and name CA) (segid 3A4 and resid 263 and name CA)	6.27	0.10	0.10
	assign (segid 3A4 and resid 259 and name CA) (segid 3A4 and resid 263 and name CB)	6.00	0.11	0.10
	assign (segid 3A4 and resid 259 and name CA) (segid 3A4 and resid 263 and name CG)	5.33	0.24	0.24
	assign (segid 3A4 and resid 259 and name CA) (segid 3A4 and resid 263 and name N)	5.22	0.07	0.07
30	assign (segid 3A4 and resid 259 and name CA) (segid 3A4 and resid 264 and name CA)	8.69	0.09	0.08
	assign (segid 3A4 and resid 259 and name CA) (segid 3A4 and resid 264 and name N)	7.38	0.07	0.07
	assign (segid 3A4 and resid 259 and name CA) (segid 3A4 and resid 265 and name CA)	9.83	0.16	0.16
	assign (segid 3A4 and resid 259 and name CA) (segid 3A4 and resid 266 and name CA)	10.44	0.15	0.15
	assign (segid 3A4 and resid 259 and name CA) (segid 3A4 and resid 267 and name CA)	12.49	0.23	0.23
35	assign (segid 3A4 and resid 259 and name CA) (segid 3A4 and resid 267 and name CB)	12.20	0.29	0.28
	assign (segid 3A4 and resid 259 and name CA) (segid 3A4 and resid 268 and name CA)	14.34	0.10	0.11
	assign (segid 3A4 and resid 259 and name CA) (segid 3A4 and resid 268 and name CB)	13.97	0.10	0.10
	assign (segid 3A4 and resid 259 and name CA) (segid 3A4 and resid 269 and name CA)	15.31	0.20	0.19
	assign (segid 3A4 and resid 259 and name CA) (segid 3A4 and resid 270 and name CA)	16.54	0.16	0.16
40	assign (segid 3A4 and resid 259 and name CA) (segid 3A4 and resid 270 and name CB)	15.92	0.22	0.22
	assign (segid 3A4 and resid 259 and name CA) (segid 3A4 and resid 271 and name CA)	18.37	0.22	0.22
	assign (segid 3A4 and resid 259 and name CA) (segid 3A4 and resid 271 and name CB)	17.89	0.22	0.22
	assign (segid 3A4 and resid 259 and name CA) (segid 3A4 and resid 272 and name CB)	19.37	0.31	0.31
	assign (segid 3A4 and resid 259 and name CA) (segid 3A4 and resid 276 and name CB)	19.64	0.21	0.20
45	assign (segid 3A4 and resid 259 and name CA) (segid 3A4 and resid 280 and name CB)	18.42	0.26	0.27
	assign (segid 3A4 and resid 259 and name CA) (segid 3A4 and resid 305 and name CA)	16.09	0.73	0.73
	assign (segid 3A4 and resid 259 and name CA) (segid 3A4 and resid 305 and name CB)	15.84	0.76	0.77
	assign (segid 3A4 and resid 259 and name CA) (segid 3A4 and resid 306 and name CA)	15.08	0.75	0.75
	assign (segid 3A4 and resid 259 and name CA) (segid 3A4 and resid 307 and name CA)	16.66	0.73	0.73
50	assign (segid 3A4 and resid 259 and name CA) (segid 3A4 and resid 307 and name CB)	18.11	0.72	0.72
	assign (segid 3A4 and resid 259 and name CA) (segid 3A4 and resid 308 and name CA)	14.92	0.68	0.68
	assign (segid 3A4 and resid 259 and name CA) (segid 3A4 and resid 308 and name CB)	15.06	0.68	0.68
	assign (segid 3A4 and resid 259 and name CA) (segid 3A4 and resid 309 and name CA)	11.42	0.68	0.68
	assign (segid 3A4 and resid 259 and name CA) (segid 3A4 and resid 309 and name CB)	10.98	0.74	0.73
55	assign (segid 3A4 and resid 259 and name CA) (segid 3A4 and resid 310 and name CA)	13.03	0.64	0.64
	assign (segid 3A4 and resid 259 and name CA) (segid 3A4 and resid 310 and name CB)	14.31	0.66	0.67
	assign (segid 3A4 and resid 259 and name CA) (segid 3A4 and resid 311 and name CA)	14.59	0.62	0.61
	assign (segid 3A4 and resid 259 and name CA) (segid 3A4 and resid 311 and name CB)	15.71	0.64	0.64
	assign (segid 3A4 and resid 259 and name CA) (segid 3A4 and resid 312 and name CA)	11.63	0.63	0.64
60	assign (segid 3A4 and resid 259 and name CA) (segid 3A4 and resid 312 and name CB)	10.76	0.67	0.67
	assign (segid 3A4 and resid 259 and name CA) (segid 3A4 and resid 313 and name CA)	10.10	0.57	0.57
	assign (segid 3A4 and resid 259 and name CA) (segid 3A4 and resid 313 and name CB)	9.80	0.57	0.58
	assign (segid 3A4 and resid 259 and name CA) (segid 3A4 and resid 314 and name CA)	13.73	0.52	0.52
	assign (segid 3A4 and resid 259 and name CA) (segid 3A4 and resid 314 and name CB)	14.97	0.52	0.51
65	assign (segid 3A4 and resid 259 and name CA) (segid 3A4 and resid 315 and name CA)	14.52	0.51	0.50
	assign (segid 3A4 and resid 259 and name CA) (segid 3A4 and resid 315 and name CB)	14.87	0.54	0.53
	assign (segid 3A4 and resid 259 and name CA) (segid 3A4 and resid 316 and name CA)	11.78	0.63	0.62
	assign (segid 3A4 and resid 259 and name CA) (segid 3A4 and resid 317 and name CA)	11.14	0.61	0.61
	assign (segid 3A4 and resid 259 and name CA) (segid 3A4 and resid 318 and name CA)	8.90	0.63	0.62
70	assign (segid 3A4 and resid 259 and name CA) (segid 3A4 and resid 318 and name CB)	7.46	0.66	0.66
	assign (segid 3A4 and resid 259 and name CA) (segid 3A4 and resid 319 and name CA)	10.63	0.65	0.65
	assign (segid 3A4 and resid 259 and name CA) (segid 3A4 and resid 319 and name CB)	10.30	0.65	0.66
	assign (segid 3A4 and resid 259 and name CA) (segid 3A4 and resid 347 and name CA)	16.33	0.61	0.61
	assign (segid 3A4 and resid 259 and name CA) (segid 3A4 and resid 347 and name CB)	15.02	0.60	0.60
75	assign (segid 3A4 and resid 259 and name CA) (segid 3A4 and resid 348 and name CA)	16.05	0.79	0.80
	assign (segid 3A4 and resid 259 and name CA) (segid 3A4 and resid 351 and name CA)	17.93	0.37	0.38
	assign (segid 3A4 and resid 259 and name CA) (segid 3A4 and resid 363 and name CA)	18.88	0.55	0.55
	assign (segid 3A4 and resid 259 and name CA) (segid 3A4 and resid 363 and name CB)	18.10	0.47	0.48
	assign (segid 3A4 and resid 259 and name CA) (segid 3A4 and resid 365 and name CB)	18.63	0.76	0.76
80	assign (segid 3A4 and resid 259 and name CA) (segid 3A4 and resid 381 and name CA)	16.70	0.39	0.38
	assign (segid 3A4 and resid 259 and name CA) (segid 3A4 and resid 382 and name CA)	15.47	0.19	0.20
	assign (segid 3A4 and resid 259 and name CA) (segid 3A4 and resid 382 and name CB)	16.56	0.17	0.18
	assign (segid 3A4 and resid 259 and name CA) (segid 3A4 and resid 383 and name CA)	11.80	0.19	0.18

5	assign	(segid 3A4 and resid 259 and name CA)	(segid 3A4 and resid 384 and name CA)	11.41	0.19	0.19
	assign	(segid 3A4 and resid 259 and name CA)	(segid 3A4 and resid 384 and name CB)	11.38	0.23	0.22
	assign	(segid 3A4 and resid 259 and name CA)	(segid 3A4 and resid 385 and name CA)	14.70	0.15	0.14
	assign	(segid 3A4 and resid 259 and name CA)	(segid 3A4 and resid 386 and name CA)	18.04	0.21	0.21
	assign	(segid 3A4 and resid 259 and name CA)	(segid 3A4 and resid 389 and name CA)	17.91	0.14	0.15
10	assign	(segid 3A4 and resid 259 and name CA)	(segid 3A4 and resid 389 and name CB)	18.11	0.31	0.31
	assign	(segid 3A4 and resid 259 and name CA)	(segid 3A4 and resid 390 and name CA)	15.59	0.25	0.25
	assign	(segid 3A4 and resid 259 and name CA)	(segid 3A4 and resid 390 and name CB)	16.20	0.37	0.38
	assign	(segid 3A4 and resid 259 and name CA)	(segid 3A4 and resid 391 and name CA)	12.19	0.24	0.23
	assign	(segid 3A4 and resid 259 and name CA)	(segid 3A4 and resid 391 and name CB)	10.87	0.24	0.25
15	assign	(segid 3A4 and resid 259 and name CA)	(segid 3A4 and resid 392 and name CA)	13.24	0.21	0.22
	assign	(segid 3A4 and resid 259 and name CA)	(segid 3A4 and resid 392 and name CB)	13.88	0.25	0.25
	assign	(segid 3A4 and resid 259 and name CA)	(segid 3A4 and resid 393 and name CA)	10.08	0.24	0.24
	assign	(segid 3A4 and resid 259 and name CA)	(segid 3A4 and resid 394 and name CA)	10.04	0.29	0.29
	assign	(segid 3A4 and resid 259 and name CA)	(segid 3A4 and resid 394 and name CB)	11.20	0.34	0.34
20	assign	(segid 3A4 and resid 259 and name CA)	(segid 3A4 and resid 395 and name CA)	11.72	0.31	0.31
	assign	(segid 3A4 and resid 259 and name CA)	(segid 3A4 and resid 396 and name CA)	9.67	0.38	0.37
	assign	(segid 3A4 and resid 259 and name CA)	(segid 3A4 and resid 396 and name CB)	9.68	0.41	0.41
	assign	(segid 3A4 and resid 259 and name CA)	(segid 3A4 and resid 397 and name C)	6.94	0.29	0.30
	assign	(segid 3A4 and resid 259 and name CA)	(segid 3A4 and resid 397 and name CA)	6.40	0.32	0.32
25	assign	(segid 3A4 and resid 259 and name CA)	(segid 3A4 and resid 397 and name CB)	6.03	0.33	0.34
	assign	(segid 3A4 and resid 259 and name CA)	(segid 3A4 and resid 397 and name O)	6.49	0.29	0.29
	assign	(segid 3A4 and resid 259 and name CA)	(segid 3A4 and resid 398 and name CA)	8.95	0.32	0.31
	assign	(segid 3A4 and resid 259 and name CA)	(segid 3A4 and resid 398 and name CB)	10.19	0.35	0.35
	assign	(segid 3A4 and resid 259 and name CA)	(segid 3A4 and resid 399 and name CA)	10.59	0.32	0.31
30	assign	(segid 3A4 and resid 259 and name CA)	(segid 3A4 and resid 399 and name CB)	11.28	0.35	0.35
	assign	(segid 3A4 and resid 259 and name CA)	(segid 3A4 and resid 400 and name CA)	8.11	0.42	0.43
	assign	(segid 3A4 and resid 259 and name CA)	(segid 3A4 and resid 400 and name CB)	6.98	0.53	0.52
	assign	(segid 3A4 and resid 259 and name CA)	(segid 3A4 and resid 401 and name CA)	7.58	0.29	0.30
	assign	(segid 3A4 and resid 259 and name CA)	(segid 3A4 and resid 402 and name CA)	11.33	0.31	0.31
35	assign	(segid 3A4 and resid 259 and name CA)	(segid 3A4 and resid 402 and name CB)	12.14	0.32	0.32
	assign	(segid 3A4 and resid 259 and name CA)	(segid 3A4 and resid 403 and name CA)	12.39	0.23	0.23
	assign	(segid 3A4 and resid 259 and name CA)	(segid 3A4 and resid 403 and name CB)	12.29	0.24	0.23
	assign	(segid 3A4 and resid 259 and name CA)	(segid 3A4 and resid 404 and name CA)	10.88	0.28	0.27
	assign	(segid 3A4 and resid 259 and name CA)	(segid 3A4 and resid 404 and name CB)	9.49	0.28	0.27
40	assign	(segid 3A4 and resid 259 and name CA)	(segid 3A4 and resid 405 and name CA)	12.24	0.55	0.54
	assign	(segid 3A4 and resid 259 and name CA)	(segid 3A4 and resid 405 and name CB)	11.90	0.58	0.57
	assign	(segid 3A4 and resid 259 and name CA)	(segid 3A4 and resid 406 and name CA)	15.40	0.51	0.50
	assign	(segid 3A4 and resid 259 and name CA)	(segid 3A4 and resid 407 and name CA)	16.08	0.31	0.32
	assign	(segid 3A4 and resid 259 and name CA)	(segid 3A4 and resid 407 and name CB)	15.61	0.31	0.30
45	assign	(segid 3A4 and resid 259 and name CA)	(segid 3A4 and resid 408 and name CA)	15.49	0.25	0.25
	assign	(segid 3A4 and resid 259 and name CA)	(segid 3A4 and resid 408 and name CB)	14.33	0.23	0.24
	assign	(segid 3A4 and resid 259 and name CA)	(segid 3A4 and resid 409 and name CA)	17.77	0.45	0.44
	assign	(segid 3A4 and resid 259 and name CA)	(segid 3A4 and resid 409 and name CB)	17.56	0.54	0.55
	assign	(segid 3A4 and resid 259 and name CA)	(segid 3A4 and resid 425 and name CA)	17.76	0.61	0.61
50	assign	(segid 3A4 and resid 259 and name CA)	(segid 3A4 and resid 426 and name CA)	16.16	1.10	1.10
	assign	(segid 3A4 and resid 259 and name CA)	(segid 3A4 and resid 427 and name CA)	15.11	0.78	0.77
	assign	(segid 3A4 and resid 259 and name CA)	(segid 3A4 and resid 428 and name CA)	16.37	0.92	0.92
	assign	(segid 3A4 and resid 259 and name CA)	(segid 3A4 and resid 429 and name CA)	15.99	1.07	1.07
	assign	(segid 3A4 and resid 259 and name CA)	(segid 3A4 and resid 430 and name CA)	16.27	1.34	1.33

	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 263 and name CA)	7.01	0.13	0.13
	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 263 and name CB)	6.47	0.13	0.13
	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 263 and name CG)	5.55	0.25	0.24
	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 263 and name N)	6.18	0.08	0.08
5	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 264 and name CA)	9.70	0.10	0.09
	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 265 and name CA)	11.09	0.13	0.13
	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 266 and name CA)	11.39	0.16	0.16
	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 267 and name CA)	13.30	0.30	0.29
	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 267 and name CB)	12.93	0.35	0.35
10	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 268 and name CA)	15.42	0.14	0.14
	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 268 and name CB)	15.14	0.10	0.10
	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 269 and name CA)	16.39	0.18	0.18
	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 270 and name CA)	17.36	0.25	0.26
	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 270 and name CB)	16.64	0.32	0.32
15	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 271 and name CA)	19.24	0.30	0.30
	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 271 and name CB)	18.78	0.29	0.29
	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 280 and name CB)	18.70	0.24	0.24
	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 305 and name CA)	16.14	0.70	0.70
	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 305 and name CB)	15.78	0.74	0.75
20	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 306 and name CA)	15.08	0.72	0.72
	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 307 and name CA)	16.97	0.69	0.69
	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 307 and name CB)	18.43	0.68	0.69
	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 308 and name CA)	15.41	0.62	0.61
	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 308 and name CB)	15.51	0.62	0.61
25	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 309 and name CA)	11.84	0.61	0.61
	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 309 and name CB)	11.21	0.65	0.65
	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 310 and name CA)	13.55	0.60	0.60
	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 310 and name CB)	14.76	0.63	0.63
	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 311 and name CA)	15.40	0.58	0.58
30	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 311 and name CB)	16.50	0.59	0.60
	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 312 and name CA)	12.61	0.59	0.59
	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 312 and name CB)	11.68	0.62	0.61
	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 313 and name CA)	11.08	0.57	0.56
	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 313 and name CB)	10.62	0.55	0.56
35	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 314 and name CA)	14.77	0.53	0.52
	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 314 and name CB)	15.94	0.51	0.51
	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 315 and name CA)	15.75	0.52	0.52
	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 315 and name CB)	16.08	0.52	0.52
	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 316 and name CA)	13.15	0.65	0.65
40	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 317 and name CA)	12.43	0.64	0.64
	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 318 and name CA)	10.28	0.62	0.61
	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 318 and name CB)	8.87	0.65	0.64
	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 319 and name CA)	11.77	0.69	0.68
	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 319 and name CB)	11.30	0.71	0.71
45	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 347 and name CA)	17.39	0.64	0.64
	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 347 and name CB)	16.04	0.63	0.62
	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 348 and name CA)	17.31	0.83	0.83
	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 351 and name CA)	19.01	0.40	0.41
	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 363 and name CB)	19.19	0.49	0.49
50	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 381 and name CA)	17.43	0.41	0.41
	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 382 and name CA)	16.19	0.24	0.23
	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 382 and name CB)	17.31	0.21	0.21
	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 383 and name CA)	12.61	0.21	0.21
	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 384 and name CA)	11.84	0.24	0.23
55	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 384 and name CB)	11.64	0.28	0.28
	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 385 and name CA)	15.18	0.18	0.18
	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 386 and name CA)	18.38	0.26	0.25
	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 389 and name CA)	17.93	0.15	0.15
	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 389 and name CB)	18.21	0.28	0.29
60	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 390 and name CA)	15.62	0.28	0.29
	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 390 and name CB)	16.21	0.40	0.39
	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 391 and name CA)	12.06	0.27	0.28
	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 391 and name CB)	10.82	0.28	0.29
	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 392 and name CA)	12.69	0.23	0.23
65	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 392 and name CB)	13.27	0.25	0.24
	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 393 and name CA)	9.33	0.26	0.26
	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 394 and name CA)	9.60	0.36	0.37
	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 394 and name CB)	10.89	0.41	0.40
	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 395 and name CA)	10.94	0.40	0.40
70	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 396 and name CA)	8.55	0.44	0.43
	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 396 and name CB)	8.46	0.44	0.45
	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 397 and name CA)	6.28	0.38	0.39
	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 397 and name CB)	5.61	0.41	0.40
	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 397 and name N)	5.50	0.42	0.42
75	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 397 and name O)	6.66	0.42	0.42
	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 398 and name CA)	5.87	0.37	0.38
	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 398 and name CB)	8.47	0.40	0.39
	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 399 and name CA)	9.78	0.42	0.41
	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 399 and name CB)	9.69	0.39	0.40
80	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 399 and name CB)	10.25	0.41	0.41
	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 400 and name C)	7.11	0.37	0.37
	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 400 and name CA)	7.11	0.46	0.45
	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 400 and name CB)	5.84	0.54	0.53

	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 401 and name CA)	7.24	0.34	0.34
	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 401 and name N)	6.81	0.35	0.35
	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 402 and name CA)	10.94	0.35	0.34
	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 402 and name CB)	11.68	0.35	0.36
	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 403 and name CA)	11.67	0.28	0.27
5	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 403 and name CB)	11.40	0.27	0.28
	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 404 and name CA)	10.38	0.29	0.30
	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 404 and name CB)	9.05	0.30	0.30
	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 405 and name CA)	12.15	0.51	0.51
	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 405 and name CB)	11.92	0.51	0.52
10	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 406 and name CA)	15.10	0.47	0.46
	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 407 and name CA)	15.63	0.33	0.34
	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 407 and name CB)	15.04	0.32	0.33
	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 408 and name CA)	15.33	0.22	0.21
	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 408 and name CB)	14.27	0.20	0.21
15	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 409 and name CA)	17.78	0.43	0.44
	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 409 and name CB)	17.64	0.55	0.55
	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 425 and name CA)	19.07	0.65	0.64
	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 426 and name CA)	17.56	1.11	1.11
	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 427 and name CA)	16.48	0.83	0.83
20	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 428 and name CA)	17.72	0.88	0.89
	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 431 and name CA)	15.17	0.76	0.75
	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 433 and name CA)	12.68	0.50	0.49
	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 434 and name CA)	11.66	0.54	0.54
	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 435 and name CA)	13.20	0.66	0.66
25	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 436 and name CA)	14.94	1.40	1.40
	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 437 and name CA)	16.37	1.08	1.08
	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 438 and name CA)	16.50	0.88	0.88
	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 439 and name CA)	19.05	0.33	0.32
30	assign (segid 3A4 and resid 259 and name CB)	(segid HEM and resid 1 and name C1C)	6.30	0.23	0.23
	assign (segid 3A4 and resid 259 and name CB)	(segid HEM and resid 1 and name C2B)	7.06	0.19	0.20
	assign (segid 3A4 and resid 259 and name CB)	(segid HEM and resid 1 and name C2C)	6.15	0.22	0.21
	assign (segid 3A4 and resid 259 and name CB)	(segid HEM and resid 1 and name C3B)	5.86	0.21	0.21
	assign (segid 3A4 and resid 259 and name CB)	(segid HEM and resid 1 and name C3C)	7.38	0.21	0.21
35	assign (segid 3A4 and resid 259 and name CB)	(segid HEM and resid 1 and name C4B)	6.16	0.25	0.24
	assign (segid 3A4 and resid 259 and name CB)	(segid HEM and resid 1 and name CAB)	4.76	0.18	0.19
	assign (segid 3A4 and resid 259 and name CB)	(segid HEM and resid 1 and name CBB)	4.86	0.20	0.19
	assign (segid 3A4 and resid 259 and name CB)	(segid HEM and resid 1 and name CHC)	5.54	0.23	0.22
	assign (segid 3A4 and resid 259 and name CB)	(segid HEM and resid 1 and name CMC)	5.13	0.20	0.20
	assign (segid 3A4 and resid 259 and name CB)	(segid HEM and resid 1 and name NB)	7.45	0.26	0.26
40	assign (segid 3A4 and resid 259 and name CB)	(segid 3A4 and resid 259 and name C)	2.47	0.01	0.01
	assign (segid 3A4 and resid 259 and name N)	(segid 3A4 and resid 259 and name CA)	1.46	0.01	0.02
	assign (segid 3A4 and resid 259 and name N)	(segid 3A4 and resid 259 and name CB)	2.45	0.02	0.02
	assign (segid 3A4 and resid 259 and name N)	(segid 3A4 and resid 259 and name O)	3.52	0.03	0.02
	assign (segid 3A4 and resid 259 and name N)	(segid 3A4 and resid 260 and name C)	4.73	0.05	0.05
45	assign (segid 3A4 and resid 259 and name N)	(segid 3A4 and resid 260 and name CA)	4.23	0.06	0.05
	assign (segid 3A4 and resid 259 and name N)	(segid 3A4 and resid 260 and name CB)	4.96	0.13	0.13
	assign (segid 3A4 and resid 259 and name N)	(segid 3A4 and resid 260 and name N)	2.81	0.05	0.06
	assign (segid 3A4 and resid 259 and name N)	(segid 3A4 and resid 260 and name O)	5.78	0.05	0.05
	assign (segid 3A4 and resid 259 and name N)	(segid 3A4 and resid 261 and name C)	5.64	0.09	0.09
50	assign (segid 3A4 and resid 259 and name N)	(segid 3A4 and resid 261 and name CA)	5.39	0.12	0.11
	assign (segid 3A4 and resid 259 and name N)	(segid 3A4 and resid 261 and name N)	4.39	0.09	0.08
	assign (segid 3A4 and resid 259 and name N)	(segid 3A4 and resid 261 and name O)	6.83	0.09	0.09
	assign (segid 3A4 and resid 259 and name N)	(segid 3A4 and resid 262 and name C)	6.50	0.05	0.05
	assign (segid 3A4 and resid 259 and name N)	(segid 3A4 and resid 262 and name CA)	5.60	0.07	0.07
55	assign (segid 3A4 and resid 259 and name N)	(segid 3A4 and resid 262 and name CB)	5.03	0.07	0.07
	assign (segid 3A4 and resid 259 and name N)	(segid 3A4 and resid 262 and name N)	4.84	0.10	0.10
	assign (segid 3A4 and resid 259 and name N)	(segid 3A4 and resid 262 and name O)	7.68	0.05	0.06
	assign (segid 3A4 and resid 259 and name N)	(segid 3A4 and resid 263 and name CA)	7.37	0.08	0.07
60	assign (segid 3A4 and resid 259 and name N)	(segid 3A4 and resid 263 and name CB)	7.20	0.09	0.09
	assign (segid 3A4 and resid 259 and name N)	(segid 3A4 and resid 263 and name CG)	6.68	0.24	0.25
	assign (segid 3A4 and resid 259 and name N)	(segid 3A4 and resid 263 and name N)	6.19	0.06	0.06
	assign (segid 3A4 and resid 259 and name N)	(segid 3A4 and resid 397 and name CA)	7.06	0.34	0.33
	assign (segid 3A4 and resid 259 and name N)	(segid 3A4 and resid 397 and name CB)	6.46	0.34	0.33
65	assign (segid 3A4 and resid 259 and name N)	(segid HEM and resid 1 and name C1B)	6.68	0.20	0.21
	assign (segid 3A4 and resid 259 and name N)	(segid HEM and resid 1 and name C1C)	6.11	0.20	0.20
	assign (segid 3A4 and resid 259 and name N)	(segid HEM and resid 1 and name C2B)	5.83	0.17	0.17
	assign (segid 3A4 and resid 259 and name N)	(segid HEM and resid 1 and name C2C)	6.39	0.19	0.20
	assign (segid 3A4 and resid 259 and name N)	(segid HEM and resid 1 and name C3B)	4.92	0.17	0.16
	assign (segid 3A4 and resid 259 and name N)	(segid HEM and resid 1 and name C3C)	7.54	0.19	0.19
70	assign (segid 3A4 and resid 259 and name N)	(segid HEM and resid 1 and name C4B)	5.37	0.20	0.20
	assign (segid 3A4 and resid 259 and name N)	(segid HEM and resid 1 and name CAB)	4.10	0.13	0.13
	assign (segid 3A4 and resid 259 and name N)	(segid HEM and resid 1 and name CBB)	4.22	0.25	0.25
	assign (segid 3A4 and resid 259 and name N)	(segid HEM and resid 1 and name CHC)	5.19	0.18	0.19
	assign (segid 3A4 and resid 259 and name N)	(segid HEM and resid 1 and name CHB)	6.35	0.18	0.18
75	assign (segid 3A4 and resid 259 and name N)	(segid HEM and resid 1 and name CHC)	5.91	0.20	0.20
	assign (segid 3A4 and resid 259 and name N)	(segid HEM and resid 1 and name NB)	6.46	0.23	0.23
	assign (segid 3A4 and resid 259 and name N)	(segid HEM and resid 1 and name NC)	7.17	0.23	0.22
	assign (segid 3A4 and resid 259 and name O)	(segid 3A4 and resid 260 and name CB)	3.27	0.03	0.02
80	assign (segid 3A4 and resid 259 and name O)	(segid 3A4 and resid 260 and name C)	2.96	0.06	0.05
	assign (segid 3A4 and resid 259 and name O)	(segid 3A4 and resid 260 and name CA)	2.76	0.06	0.06
	assign (segid 3A4 and resid 259 and name O)	(segid 3A4 and resid 260 and name CB)	4.25	0.07	0.07
	assign (segid 3A4 and resid 259 and name O)	(segid 3A4 and resid 260 and name N)	2.25	0.02	0.02

	assign (segid 3A4 and resid 259 and name O) (segid 3A4 and resid 260 and name O)	3.37	0.08	0.09
	assign (segid 3A4 and resid 259 and name O) (segid 3A4 and resid 261 and name C)	4.13	0.12	0.12
	assign (segid 3A4 and resid 259 and name O) (segid 3A4 and resid 261 and name CA)	4.42	0.10	0.11
	assign (segid 3A4 and resid 259 and name O) (segid 3A4 and resid 261 and name N)	3.49	0.08	0.08
	assign (segid 3A4 and resid 259 and name O) (segid 3A4 and resid 261 and name O)	5.02	0.17	0.18
5	assign (segid 3A4 and resid 259 and name O) (segid 3A4 and resid 262 and name C)	3.88	0.04	0.03
	assign (segid 3A4 and resid 259 and name O) (segid 3A4 and resid 262 and name CA)	3.78	0.04	0.04
	assign (segid 3A4 and resid 259 and name O) (segid 3A4 and resid 262 and name CB)	3.64	0.11	0.10
	assign (segid 3A4 and resid 259 and name O) (segid 3A4 and resid 262 and name N)	3.33	0.05	0.06
	assign (segid 3A4 and resid 259 and name O) (segid 3A4 and resid 262 and name O)	5.06	0.05	0.06
10	assign (segid 3A4 and resid 259 and name O) (segid 3A4 and resid 263 and name C)	5.12	0.08	0.07
	assign (segid 3A4 and resid 259 and name O) (segid 3A4 and resid 263 and name CA)	3.98	0.08	0.08
	assign (segid 3A4 and resid 259 and name O) (segid 3A4 and resid 263 and name CB)	3.69	0.09	0.08
	assign (segid 3A4 and resid 259 and name O) (segid 3A4 and resid 263 and name CG)	3.32	0.22	0.22
	assign (segid 3A4 and resid 259 and name O) (segid 3A4 and resid 263 and name N)	3.06	0.05	0.06
15	assign (segid 3A4 and resid 259 and name O) (segid 3A4 and resid 263 and name O)	6.26	0.09	0.09
	assign (segid 3A4 and resid 259 and name O) (segid 3A4 and resid 264 and name C)	7.30	0.09	0.09
	assign (segid 3A4 and resid 259 and name O) (segid 3A4 and resid 264 and name CA)	6.46	0.10	0.10
	assign (segid 3A4 and resid 259 and name O) (segid 3A4 and resid 264 and name N)	5.10	0.09	0.09
	assign (segid 3A4 and resid 259 and name O) (segid 3A4 and resid 265 and name N)	6.94	0.14	0.13
20	assign (segid 3A4 and resid 259 and name O) (segid 3A4 and resid 266 and name N)	7.73	0.13	0.13
	assign (segid 3A4 and resid 259 and name O) (segid 3A4 and resid 266 and name O)	7.08	0.32	0.33
	assign (segid 3A4 and resid 259 and name O) (segid 3A4 and resid 267 and name CA)	6.88	0.38	0.39
	assign (segid 3A4 and resid 259 and name O) (segid 3A4 and resid 267 and name N)	7.09	0.35	0.35
	assign (segid 3A4 and resid 259 and name O) (segid 3A4 and resid 267 and name O)	7.38	0.21	0.20
25	assign (segid 3A4 and resid 259 and name O) (segid 3A4 and resid 267 and name CA)	6.13	0.20	0.20
	assign (segid 3A4 and resid 259 and name O) (segid 3A4 and resid 267 and name CB)	5.51	0.26	0.26
	assign (segid 3A4 and resid 259 and name O) (segid 3A4 and resid 267 and name N)	1.23	0.01	0.00
	assign (segid 3A4 and resid 259 and name O) (segid 3A4 and resid 267 and name O)	3.09	0.16	0.16
	assign (segid 3A4 and resid 259 and name O) (segid 3A4 and resid 267 and name CA)	2.44	0.02	0.01
30	assign (segid 3A4 and resid 259 and name O) (segid 3A4 and resid 267 and name N)	1.33	0.01	0.01
	assign (segid 3A4 and resid 259 and name O) (segid 3A4 and resid 267 and name O)	3.83	0.27	0.26
	assign (segid 3A4 and resid 259 and name O) (segid 3A4 and resid 267 and name CA)	6.64	0.75	0.75
	assign (segid 3A4 and resid 259 and name O) (segid 3A4 and resid 267 and name N)	6.07	0.87	0.87
	assign (segid 3A4 and resid 259 and name O) (segid 3A4 and resid 267 and name O)	1.53	0.01	0.01
35	assign (segid 3A4 and resid 259 and name O) (segid 3A4 and resid 267 and name CA)	2.40	0.02	0.02
	assign (segid 3A4 and resid 259 and name O) (segid 3A4 and resid 267 and name N)	4.48	0.09	0.09
	assign (segid 3A4 and resid 259 and name O) (segid 3A4 and resid 267 and name O)	3.80	0.04	0.05
	assign (segid 3A4 and resid 259 and name O) (segid 3A4 and resid 267 and name CA)	2.43	0.06	0.06
	assign (segid 3A4 and resid 259 and name O) (segid 3A4 and resid 267 and name N)	5.12	0.34	0.35
40	assign (segid 3A4 and resid 259 and name O) (segid 3A4 and resid 267 and name O)	6.44	0.45	0.46
	assign (segid 3A4 and resid 259 and name O) (segid 3A4 and resid 267 and name CA)	6.14	0.61	0.60
	assign (segid 3A4 and resid 259 and name O) (segid 3A4 and resid 267 and name N)	7.78	0.71	0.72
	assign (segid 3A4 and resid 259 and name O) (segid 3A4 and resid 267 and name O)	10.58	0.67	0.66
	assign (segid 3A4 and resid 259 and name O) (segid 3A4 and resid 267 and name CA)	11.92	0.63	0.63
45	assign (segid 3A4 and resid 259 and name O) (segid 3A4 and resid 267 and name N)	13.96	1.46	1.45
	assign (segid 3A4 and resid 259 and name O) (segid 3A4 and resid 267 and name O)	15.62	1.37	1.38
	assign (segid 3A4 and resid 259 and name O) (segid 3A4 and resid 267 and name CA)	16.50	1.35	1.35
	assign (segid 3A4 and resid 259 and name O) (segid 3A4 and resid 267 and name N)	15.60	1.23	1.24
	assign (segid 3A4 and resid 259 and name O) (segid 3A4 and resid 267 and name O)	15.69	1.31	1.31
50	assign (segid 3A4 and resid 259 and name O) (segid 3A4 and resid 267 and name CA)	17.77	1.02	1.03
	assign (segid 3A4 and resid 259 and name O) (segid 3A4 and resid 267 and name N)	17.47	0.93	0.93
	assign (segid 3A4 and resid 259 and name O) (segid 3A4 and resid 267 and name O)	11.56	0.90	0.90
	assign (segid 3A4 and resid 259 and name O) (segid 3A4 and resid 267 and name CA)	10.92	0.91	0.91
	assign (segid 3A4 and resid 259 and name O) (segid 3A4 and resid 267 and name N)	17.13	0.68	0.67
55	assign (segid 3A4 and resid 259 and name O) (segid 3A4 and resid 267 and name O)	16.94	0.97	0.97
	assign (segid 3A4 and resid 259 and name O) (segid 3A4 and resid 267 and name CA)	17.54	0.61	0.61
	assign (segid 3A4 and resid 259 and name O) (segid 3A4 and resid 267 and name N)	17.05	0.58	0.59
	assign (segid 3A4 and resid 259 and name O) (segid 3A4 and resid 267 and name O)	18.57	0.79	0.80
	assign (segid 3A4 and resid 259 and name O) (segid 3A4 and resid 267 and name CA)	15.30	0.92	0.91
60	assign (segid 3A4 and resid 259 and name O) (segid 3A4 and resid 267 and name N)	16.14	0.91	0.92
	assign (segid 3A4 and resid 259 and name O) (segid 3A4 and resid 267 and name O)	16.01	0.87	0.87
	assign (segid 3A4 and resid 259 and name O) (segid 3A4 and resid 267 and name CA)	13.18	0.89	0.89
	assign (segid 3A4 and resid 259 and name O) (segid 3A4 and resid 267 and name N)	13.42	0.86	0.87
	assign (segid 3A4 and resid 259 and name O) (segid 3A4 and resid 267 and name O)	11.40	1.15	1.14
65	assign (segid 3A4 and resid 259 and name O) (segid 3A4 and resid 267 and name CA)	12.33	1.06	1.06
	assign (segid 3A4 and resid 259 and name O) (segid 3A4 and resid 267 and name N)	13.78	1.03	1.03
	assign (segid 3A4 and resid 259 and name O) (segid 3A4 and resid 267 and name O)	11.92	1.20	1.19
	assign (segid 3A4 and resid 259 and name O) (segid 3A4 and resid 267 and name CA)	10.65	1.22	1.22
	assign (segid 3A4 and resid 259 and name O) (segid 3A4 and resid 267 and name N)	15.32	1.22	1.21
70	assign (segid 3A4 and resid 259 and name O) (segid 3A4 and resid 267 and name O)	16.57	1.22	1.21
	assign (segid 3A4 and resid 259 and name O) (segid 3A4 and resid 267 and name CA)	15.66	1.16	1.15
	assign (segid 3A4 and resid 259 and name O) (segid 3A4 and resid 267 and name N)	15.12	1.09	1.09
	assign (segid 3A4 and resid 259 and name O) (segid 3A4 and resid 267 and name O)	16.98	1.14	1.13
	assign (segid 3A4 and resid 259 and name O) (segid 3A4 and resid 267 and name CA)	16.63	1.15	1.15
75	assign (segid 3A4 and resid 259 and name O) (segid 3A4 and resid 267 and name N)	14.24	2.31	2.32
	assign (segid 3A4 and resid 259 and name O) (segid 3A4 and resid 267 and name O)	15.47	1.83	1.84
	assign (segid 3A4 and resid 259 and name O) (segid 3A4 and resid 267 and name CA)	12.04	3.16	3.17
	assign (segid 3A4 and resid 259 and name O) (segid 3A4 and resid 267 and name N)	2.42	0.02	0.02
	assign (segid 3A4 and resid 259 and name O) (segid 3A4 and resid 267 and name O)	1.46	0.01	0.00
80	assign (segid 3A4 and resid 259 and name O) (segid 3A4 and resid 267 and name CA)	2.81	0.24	0.23
	assign (segid 3A4 and resid 259 and name O) (segid 3A4 and resid 267 and name N)	5.09	0.20	0.20
	assign (segid 3A4 and resid 259 and name O) (segid 3A4 and resid 267 and name O)	4.70	0.20	0.21

	assign (segid 3A4 and resid 25 and name N) (segid 3A4 and resid 26 and name N)	3.46	0.25	0.26
	assign (segid 3A4 and resid 25 and name N) (segid 3A4 and resid 26 and name O)	5.68	0.37	0.38
	assign (segid 3A4 and resid 25 and name N) (segid 3A4 and resid 29 and name C)	5.95	0.30	0.31
	assign (segid 3A4 and resid 25 and name N) (segid 3A4 and resid 29 and name CA)	5.30	0.30	0.29
	assign (segid 3A4 and resid 25 and name N) (segid 3A4 and resid 29 and name N)	5.19	0.39	0.39
5	assign (segid 3A4 and resid 25 and name N) (segid 3A4 and resid 29 and name O)	6.85	0.32	0.33
	assign (segid 3A4 and resid 25 and name N) (segid 3A4 and resid 30 and name CA)	6.84	0.55	0.55
	assign (segid 3A4 and resid 25 and name N) (segid 3A4 and resid 30 and name N)	5.85	0.40	0.41
	assign (segid 3A4 and resid 25 and name N) (segid 3A4 and resid 30 and name O)	7.00	0.43	0.44
	assign (segid 3A4 and resid 25 and name N) (segid 3A4 and resid 26 and name C)	3.08	0.32	0.32
10	assign (segid 3A4 and resid 25 and name O) (segid 3A4 and resid 26 and name CA)	2.77	0.02	0.03
	assign (segid 3A4 and resid 25 and name O) (segid 3A4 and resid 26 and name N)	2.24	0.01	0.01
	assign (segid 3A4 and resid 25 and name O) (segid 3A4 and resid 26 and name O)	3.78	0.41	0.41
	assign (segid 3A4 and resid 25 and name O) (segid 3A4 and resid 29 and name C)	6.81	0.98	0.98
	assign (segid 3A4 and resid 25 and name O) (segid 3A4 and resid 29 and name CA)	6.16	1.00	1.00
15	assign (segid 3A4 and resid 25 and name O) (segid 3A4 and resid 29 and name N)	5.52	1.05	1.05
	assign (segid 3A4 and resid 25 and name O) (segid 3A4 and resid 260 and name CB)	2.49	0.04	0.03
	assign (segid 3A4 and resid 260 and name C) (segid 3A4 and resid 260 and name O)	1.23	0.00	0.01
	assign (segid 3A4 and resid 260 and name C) (segid 3A4 and resid 261 and name C)	3.03	0.05	0.05
	assign (segid 3A4 and resid 260 and name C) (segid 3A4 and resid 261 and name N)	2.44	0.01	0.02
20	assign (segid 3A4 and resid 260 and name C) (segid 3A4 and resid 261 and name O)	1.34	0.01	0.00
	assign (segid 3A4 and resid 260 and name C) (segid 3A4 and resid 262 and name C)	3.88	0.12	0.12
	assign (segid 3A4 and resid 260 and name C) (segid 3A4 and resid 262 and name CA)	4.60	0.12	0.13
	assign (segid 3A4 and resid 260 and name C) (segid 3A4 and resid 262 and name CB)	4.47	0.12	0.12
	assign (segid 3A4 and resid 260 and name C) (segid 3A4 and resid 262 and name N)	5.20	0.14	0.13
25	assign (segid 3A4 and resid 260 and name C) (segid 3A4 and resid 262 and name O)	3.28	0.14	0.14
	assign (segid 3A4 and resid 260 and name C) (segid 3A4 and resid 263 and name C)	5.69	0.15	0.16
	assign (segid 3A4 and resid 260 and name C) (segid 3A4 and resid 263 and name CA)	5.01	0.13	0.13
	assign (segid 3A4 and resid 260 and name C) (segid 3A4 and resid 263 and name CB)	4.70	0.11	0.10
	assign (segid 3A4 and resid 260 and name C) (segid 3A4 and resid 263 and name CG)	4.53	0.11	0.11
30	assign (segid 3A4 and resid 260 and name C) (segid 3A4 and resid 263 and name N)	5.05	0.22	0.23
	assign (segid 3A4 and resid 260 and name C) (segid 3A4 and resid 263 and name O)	3.92	0.09	0.09
	assign (segid 3A4 and resid 260 and name C) (segid 3A4 and resid 264 and name C)	6.23	0.14	0.13
	assign (segid 3A4 and resid 260 and name C) (segid 3A4 and resid 264 and name CA)	6.19	0.24	0.23
	assign (segid 3A4 and resid 260 and name C) (segid 3A4 and resid 264 and name N)	5.16	0.21	0.22
35	assign (segid 3A4 and resid 260 and name C) (segid 3A4 and resid 264 and name O)	4.26	0.17	0.18
	assign (segid 3A4 and resid 260 and name C) (segid 3A4 and resid 265 and name N)	7.36	0.24	0.25
	assign (segid 3A4 and resid 260 and name CA) (segid 3A4 and resid 260 and name CB)	6.00	0.28	0.27
	assign (segid 3A4 and resid 260 and name CA) (segid 3A4 and resid 260 and name O)	1.52	0.01	0.01
40	assign (segid 3A4 and resid 260 and name CA) (segid 3A4 and resid 261 and name C)	1.54	0.02	0.01
	assign (segid 3A4 and resid 260 and name CA) (segid 3A4 and resid 261 and name CA)	2.40	0.02	0.02
	assign (segid 3A4 and resid 260 and name CA) (segid 3A4 and resid 261 and name N)	4.42	0.05	0.05
	assign (segid 3A4 and resid 260 and name CA) (segid 3A4 and resid 261 and name O)	3.81	0.00	0.01
	assign (segid 3A4 and resid 260 and name CA) (segid 3A4 and resid 262 and name C)	2.44	0.02	0.01
45	assign (segid 3A4 and resid 260 and name CA) (segid 3A4 and resid 262 and name CA)	5.34	0.13	0.12
	assign (segid 3A4 and resid 260 and name CA) (segid 3A4 and resid 262 and name CB)	5.57	0.16	0.16
	assign (segid 3A4 and resid 260 and name CA) (segid 3A4 and resid 262 and name N)	5.46	0.14	0.14
	assign (segid 3A4 and resid 260 and name CA) (segid 3A4 and resid 262 and name O)	5.86	0.17	0.16
	assign (segid 3A4 and resid 260 and name CA) (segid 3A4 and resid 263 and name C)	4.39	0.15	0.14
50	assign (segid 3A4 and resid 260 and name CA) (segid 3A4 and resid 263 and name CA)	6.72	0.17	0.18
	assign (segid 3A4 and resid 260 and name CA) (segid 3A4 and resid 263 and name CB)	5.90	0.18	0.18
	assign (segid 3A4 and resid 260 and name CA) (segid 3A4 and resid 263 and name CG)	5.33	0.15	0.16
	assign (segid 3A4 and resid 260 and name CA) (segid 3A4 and resid 263 and name N)	4.76	0.15	0.16
	assign (segid 3A4 and resid 260 and name CA) (segid 3A4 and resid 263 and name O)	4.95	0.21	0.20
55	assign (segid 3A4 and resid 260 and name CA) (segid 3A4 and resid 263 and name CA)	4.69	0.13	0.14
	assign (segid 3A4 and resid 260 and name CA) (segid 3A4 and resid 264 and name N)	7.10	0.17	0.18
	assign (segid 3A4 and resid 260 and name CA) (segid 3A4 and resid 264 and name O)	6.34	0.26	0.25
	assign (segid 3A4 and resid 260 and name CA) (segid 3A4 and resid 264 and name CA)	5.35	0.23	0.22
	assign (segid 3A4 and resid 260 and name CA) (segid 3A4 and resid 265 and name CA)	8.65	0.31	0.30
60	assign (segid 3A4 and resid 260 and name CA) (segid 3A4 and resid 266 and name CA)	9.94	0.24	0.24
	assign (segid 3A4 and resid 260 and name CA) (segid 3A4 and resid 267 and name CA)	10.96	0.19	0.18
	assign (segid 3A4 and resid 260 and name CA) (segid 3A4 and resid 267 and name CB)	10.31	0.22	0.21
	assign (segid 3A4 and resid 260 and name CA) (segid 3A4 and resid 268 and name CA)	12.58	0.17	0.17
	assign (segid 3A4 and resid 260 and name CA) (segid 3A4 and resid 268 and name CB)	12.15	0.22	0.21
65	assign (segid 3A4 and resid 260 and name CA) (segid 3A4 and resid 269 and name CA)	14.43	0.23	0.23
	assign (segid 3A4 and resid 260 and name CA) (segid 3A4 and resid 270 and name CA)	15.66	0.15	0.15
	assign (segid 3A4 and resid 260 and name CA) (segid 3A4 and resid 270 and name CB)	15.08	0.17	0.16
	assign (segid 3A4 and resid 260 and name CA) (segid 3A4 and resid 271 and name CA)	16.75	0.19	0.19
	assign (segid 3A4 and resid 260 and name CA) (segid 3A4 and resid 271 and name CB)	16.00	0.22	0.23
70	assign (segid 3A4 and resid 260 and name CA) (segid 3A4 and resid 272 and name CA)	18.54	0.26	0.26
	assign (segid 3A4 and resid 260 and name CA) (segid 3A4 and resid 272 and name CB)	18.04	0.35	0.36
	assign (segid 3A4 and resid 260 and name CA) (segid 3A4 and resid 280 and name CB)	18.72	0.56	0.56
	assign (segid 3A4 and resid 260 and name CA) (segid 3A4 and resid 305 and name CA)	17.45	0.97	0.97
	assign (segid 3A4 and resid 260 and name CA) (segid 3A4 and resid 305 and name CB)	17.12	0.99	1.00
75	assign (segid 3A4 and resid 260 and name CA) (segid 3A4 and resid 306 and name CA)	17.21	0.93	0.93
	assign (segid 3A4 and resid 260 and name CA) (segid 3A4 and resid 308 and name CA)	16.27	0.95	0.95
	assign (segid 3A4 and resid 260 and name CA) (segid 3A4 and resid 308 and name CB)	16.14	0.98	0.99
	assign (segid 3A4 and resid 260 and name CA) (segid 3A4 and resid 309 and name CA)	13.25	0.90	0.90
	assign (segid 3A4 and resid 260 and name CA) (segid 3A4 and resid 309 and name CB)	13.02	0.95	0.95
80	assign (segid 3A4 and resid 260 and name CA) (segid 3A4 and resid 310 and name CA)	15.39	0.79	0.80
	assign (segid 3A4 and resid 260 and name CA) (segid 3A4 and resid 310 and name CB)	16.79	0.79	0.79
	assign (segid 3A4 and resid 260 and name CA) (segid 3A4 and resid 311 and name CA)	16.27	0.81	0.81
	assign (segid 3A4 and resid 260 and name CA) (segid 3A4 and resid 311 and name CB)	17.19	0.86	0.85

	assign (segid 3A4 and resid 260 and name CA)	(segid 3A4 and resid 312 and name CA)	12.81	0.84	0.84
	assign (segid 3A4 and resid 260 and name CA)	(segid 3A4 and resid 312 and name CB)	11.80	0.89	0.88
	assign (segid 3A4 and resid 260 and name CA)	(segid 3A4 and resid 313 and name CA)	12.14	0.65	0.66
	assign (segid 3A4 and resid 260 and name CA)	(segid 3A4 and resid 313 and name CB)	12.26	0.65	0.64
5	assign (segid 3A4 and resid 260 and name CA)	(segid 3A4 and resid 314 and name CA)	15.66	0.59	0.58
	assign (segid 3A4 and resid 260 and name CA)	(segid 3A4 and resid 314 and name CB)	16.92	0.60	0.60
	assign (segid 3A4 and resid 260 and name CA)	(segid 3A4 and resid 315 and name CA)	15.56	0.60	0.60
	assign (segid 3A4 and resid 260 and name CA)	(segid 3A4 and resid 315 and name CB)	15.69	0.68	0.68
	assign (segid 3A4 and resid 260 and name CA)	(segid 3A4 and resid 316 and name CA)	12.46	0.63	0.63
10	assign (segid 3A4 and resid 260 and name CA)	(segid 3A4 and resid 317 and name CA)	12.64	0.62	0.61
	assign (segid 3A4 and resid 260 and name CA)	(segid 3A4 and resid 318 and name CA)	9.98	0.67	0.68
	assign (segid 3A4 and resid 260 and name CA)	(segid 3A4 and resid 318 and name CB)	8.60	0.71	0.71
	assign (segid 3A4 and resid 260 and name CA)	(segid 3A4 and resid 319 and name CA)	12.27	0.55	0.55
	assign (segid 3A4 and resid 260 and name CA)	(segid 3A4 and resid 319 and name CB)	12.33	0.51	0.52
15	assign (segid 3A4 and resid 260 and name CA)	(segid 3A4 and resid 347 and name CA)	18.43	0.68	0.69
	assign (segid 3A4 and resid 260 and name CA)	(segid 3A4 and resid 347 and name CB)	17.25	0.67	0.68
	assign (segid 3A4 and resid 260 and name CA)	(segid 3A4 and resid 348 and name CA)	17.55	0.84	0.84
	assign (segid 3A4 and resid 260 and name CA)	(segid 3A4 and resid 363 and name CB)	18.37	0.67	0.67
20	assign (segid 3A4 and resid 260 and name CA)	(segid 3A4 and resid 382 and name CA)	18.41	0.23	0.23
	assign (segid 3A4 and resid 260 and name CA)	(segid 3A4 and resid 382 and name CB)	19.42	0.25	0.25
	assign (segid 3A4 and resid 260 and name CA)	(segid 3A4 and resid 383 and name CA)	14.64	0.25	0.24
	assign (segid 3A4 and resid 260 and name CA)	(segid 3A4 and resid 384 and name CA)	14.80	0.17	0.18
	assign (segid 3A4 and resid 260 and name CA)	(segid 3A4 and resid 384 and name CB)	14.93	0.17	0.18
25	assign (segid 3A4 and resid 260 and name CA)	(segid 3A4 and resid 385 and name CA)	17.90	0.19	0.18
	assign (segid 3A4 and resid 260 and name CA)	(segid 3A4 and resid 390 and name CA)	19.12	0.21	0.21
	assign (segid 3A4 and resid 260 and name CA)	(segid 3A4 and resid 391 and name CA)	15.77	0.20	0.21
	assign (segid 3A4 and resid 260 and name CA)	(segid 3A4 and resid 391 and name CB)	14.49	0.21	0.21
	assign (segid 3A4 and resid 260 and name CA)	(segid 3A4 and resid 392 and name CA)	16.84	0.25	0.26
30	assign (segid 3A4 and resid 260 and name CA)	(segid 3A4 and resid 392 and name CB)	17.34	0.29	0.30
	assign (segid 3A4 and resid 260 and name CA)	(segid 3A4 and resid 393 and name CA)	13.68	0.28	0.27
	assign (segid 3A4 and resid 260 and name CA)	(segid 3A4 and resid 394 and name CA)	13.84	0.28	0.29
	assign (segid 3A4 and resid 260 and name CA)	(segid 3A4 and resid 394 and name CB)	15.01	0.34	0.33
	assign (segid 3A4 and resid 260 and name CA)	(segid 3A4 and resid 395 and name CA)	15.31	0.32	0.31
35	assign (segid 3A4 and resid 260 and name CA)	(segid 3A4 and resid 396 and name CA)	12.93	0.36	0.36
	assign (segid 3A4 and resid 260 and name CA)	(segid 3A4 and resid 396 and name CB)	12.86	0.39	0.39
	assign (segid 3A4 and resid 260 and name CA)	(segid 3A4 and resid 397 and name CA)	9.90	0.32	0.32
	assign (segid 3A4 and resid 260 and name CA)	(segid 3A4 and resid 397 and name CB)	9.74	0.34	0.35
	assign (segid 3A4 and resid 260 and name CA)	(segid 3A4 and resid 398 and name CA)	12.10	0.40	0.39
40	assign (segid 3A4 and resid 260 and name CA)	(segid 3A4 and resid 398 and name CB)	13.44	0.43	0.43
	assign (segid 3A4 and resid 260 and name CA)	(segid 3A4 and resid 399 and name CA)	13.22	0.31	0.32
	assign (segid 3A4 and resid 260 and name CA)	(segid 3A4 and resid 399 and name CB)	13.97	0.34	0.34
	assign (segid 3A4 and resid 260 and name CA)	(segid 3A4 and resid 400 and name CA)	10.08	0.38	0.38
	assign (segid 3A4 and resid 260 and name CA)	(segid 3A4 and resid 400 and name CB)	9.03	0.46	0.46
45	assign (segid 3A4 and resid 260 and name CA)	(segid 3A4 and resid 401 and name CA)	9.29	0.47	0.47
	assign (segid 3A4 and resid 260 and name CA)	(segid 3A4 and resid 402 and name CA)	12.98	0.48	0.49
	assign (segid 3A4 and resid 260 and name CA)	(segid 3A4 and resid 402 and name CB)	14.11	0.47	0.47
	assign (segid 3A4 and resid 260 and name CA)	(segid 3A4 and resid 403 and name CA)	13.48	0.29	0.30
	assign (segid 3A4 and resid 260 and name CA)	(segid 3A4 and resid 403 and name CB)	13.49	0.28	0.27
50	assign (segid 3A4 and resid 260 and name CA)	(segid 3A4 and resid 404 and name CA)	10.99	0.34	0.34
	assign (segid 3A4 and resid 260 and name CA)	(segid 3A4 and resid 404 and name CB)	9.50	0.33	0.32
	assign (segid 3A4 and resid 260 and name CA)	(segid 3A4 and resid 405 and name CA)	12.31	0.81	0.82
	assign (segid 3A4 and resid 260 and name CA)	(segid 3A4 and resid 405 and name CB)	12.23	0.85	0.86
	assign (segid 3A4 and resid 260 and name CA)	(segid 3A4 and resid 406 and name CA)	15.78	0.70	0.70
55	assign (segid 3A4 and resid 260 and name CA)	(segid 3A4 and resid 407 and name CA)	15.83	0.44	0.43
	assign (segid 3A4 and resid 260 and name CA)	(segid 3A4 and resid 407 and name CB)	15.35	0.41	0.40
	assign (segid 3A4 and resid 260 and name CA)	(segid 3A4 and resid 408 and name CA)	14.47	0.43	0.42
	assign (segid 3A4 and resid 260 and name CA)	(segid 3A4 and resid 408 and name CB)	13.19	0.44	0.44
	assign (segid 3A4 and resid 260 and name CA)	(segid 3A4 and resid 409 and name CA)	16.98	0.59	0.58
60	assign (segid 3A4 and resid 260 and name CA)	(segid 3A4 and resid 409 and name CB)	16.99	0.65	0.65
	assign (segid 3A4 and resid 260 and name CA)	(segid 3A4 and resid 411 and name CB)	18.64	0.46	0.45
	assign (segid 3A4 and resid 260 and name CA)	(segid 3A4 and resid 412 and name CA)	19.07	0.31	0.30
	assign (segid 3A4 and resid 260 and name CA)	(segid 3A4 and resid 414 and name CA)	18.25	0.55	0.54
	assign (segid 3A4 and resid 260 and name CA)	(segid 3A4 and resid 424 and name CA)	16.54	1.66	1.66
65	assign (segid 3A4 and resid 260 and name CA)	(segid 3A4 and resid 425 and name CA)	15.34	0.99	0.99
	assign (segid 3A4 and resid 260 and name CA)	(segid 3A4 and resid 426 and name CA)	14.06	1.12	1.12
	assign (segid 3A4 and resid 260 and name CA)	(segid 3A4 and resid 427 and name CA)	13.26	1.02	1.02
	assign (segid 3A4 and resid 260 and name CA)	(segid 3A4 and resid 428 and name CA)	14.82	0.99	0.99
	assign (segid 3A4 and resid 260 and name CA)	(segid 3A4 and resid 429 and name CA)	15.02	1.07	1.07
70	assign (segid 3A4 and resid 260 and name CA)	(segid 3A4 and resid 430 and name CA)	15.91	1.42	1.41
	assign (segid 3A4 and resid 260 and name CA)	(segid 3A4 and resid 431 and name CA)	14.31	0.56	0.57
	assign (segid 3A4 and resid 260 and name CA)	(segid 3A4 and resid 433 and name CA)	10.67	0.61	0.61
	assign (segid 3A4 and resid 260 and name CA)	(segid 3A4 and resid 434 and name CA)	8.63	0.67	0.68
	assign (segid 3A4 and resid 260 and name CA)	(segid 3A4 and resid 435 and name CA)	9.41	0.82	0.81
75	assign (segid 3A4 and resid 260 and name CA)	(segid 3A4 and resid 436 and name CA)	10.74	1.55	1.56
	assign (segid 3A4 and resid 260 and name CA)	(segid 3A4 and resid 437 and name CA)	11.95	1.15	1.15
	assign (segid 3A4 and resid 260 and name CA)	(segid 3A4 and resid 438 and name CA)	12.30	0.92	0.93
	assign (segid 3A4 and resid 260 and name CA)	(segid 3A4 and resid 439 and name CA)	14.91	0.44	0.44
	assign (segid 3A4 and resid 260 and name CA)	(segid 3A4 and resid 440 and name CA)	15.86	0.33	0.33
80	assign (segid 3A4 and resid 260 and name CB)	(segid 3A4 and resid 261 and name C)	5.39	0.05	0.05
	assign (segid 3A4 and resid 260 and name CB)	(segid 3A4 and resid 261 and name CA)	4.42	0.08	0.07
	assign (segid 3A4 and resid 260 and name CB)	(segid 3A4 and resid 261 and name N)	3.08	0.07	0.08
	assign (segid 3A4 and resid 260 and name CB)	(segid 3A4 and resid 261 and name O)	6.28	0.14	0.13
	assign (segid 3A4 and resid 260 and name CB)	(segid 3A4 and resid 262 and name C)	6.96	0.17	0.16

	assign (segid 3A4 and resid 260 and name CB)	(segid 3A4 and resid 262 and name CA)	6.79	0.10	0.10
	assign (segid 3A4 and resid 260 and name CB)	(segid 3A4 and resid 262 and name CB)	7.25	0.12	0.12
	assign (segid 3A4 and resid 260 and name CB)	(segid 3A4 and resid 262 and name N)	5.57	0.09	0.10
	assign (segid 3A4 and resid 260 and name CB)	(segid 3A4 and resid 263 and name C)	7.07	0.28	0.27
5	assign (segid 3A4 and resid 260 and name CB)	(segid 3A4 and resid 263 and name CA)	6.68	0.22	0.23
	assign (segid 3A4 and resid 260 and name CB)	(segid 3A4 and resid 263 and name CB)	6.04	0.25	0.26
	assign (segid 3A4 and resid 260 and name CB)	(segid 3A4 and resid 263 and name CG)	6.31	0.23	0.22
	assign (segid 3A4 and resid 260 and name CB)	(segid 3A4 and resid 263 and name N)	6.12	0.17	0.16
	assign (segid 3A4 and resid 260 and name CB)	(segid 3A4 and resid 264 and name CA)	7.12	0.37	0.36
10	assign (segid 3A4 and resid 260 and name CB)	(segid 3A4 and resid 264 and name N)	6.35	0.32	0.31
	assign (segid 3A4 and resid 260 and name CB)	(segid 3A4 and resid 265 and name CA)	9.61	0.36	0.36
	assign (segid 3A4 and resid 260 and name CB)	(segid 3A4 and resid 266 and name CA)	11.20	0.29	0.29
	assign (segid 3A4 and resid 260 and name CB)	(segid 3A4 and resid 267 and name CA)	11.96	0.27	0.27
	assign (segid 3A4 and resid 260 and name CB)	(segid 3A4 and resid 267 and name CB)	11.20	0.30	0.30
15	assign (segid 3A4 and resid 260 and name CB)	(segid 3A4 and resid 268 and name CA)	13.39	0.27	0.27
	assign (segid 3A4 and resid 260 and name CB)	(segid 3A4 and resid 268 and name CB)	12.88	0.31	0.30
	assign (segid 3A4 and resid 260 and name CB)	(segid 3A4 and resid 269 and name CA)	15.49	0.30	0.30
	assign (segid 3A4 and resid 260 and name CB)	(segid 3A4 and resid 270 and name CA)	16.79	0.24	0.23
	assign (segid 3A4 and resid 260 and name CB)	(segid 3A4 and resid 270 and name CB)	16.23	0.26	0.25
20	assign (segid 3A4 and resid 260 and name CB)	(segid 3A4 and resid 271 and name CA)	17.62	0.26	0.27
	assign (segid 3A4 and resid 260 and name CB)	(segid 3A4 and resid 271 and name CB)	16.78	0.31	0.31
	assign (segid 3A4 and resid 260 and name CB)	(segid 3A4 and resid 308 and name CA)	17.76	0.98	0.97
	assign (segid 3A4 and resid 260 and name CB)	(segid 3A4 and resid 308 and name CB)	17.62	1.03	1.02
	assign (segid 3A4 and resid 260 and name CB)	(segid 3A4 and resid 309 and name CA)	14.76	0.91	0.90
25	assign (segid 3A4 and resid 260 and name CB)	(segid 3A4 and resid 309 and name CB)	14.53	0.94	0.95
	assign (segid 3A4 and resid 260 and name CB)	(segid 3A4 and resid 310 and name CA)	16.85	0.77	0.78
	assign (segid 3A4 and resid 260 and name CB)	(segid 3A4 and resid 310 and name CB)	18.25	0.77	0.77
	assign (segid 3A4 and resid 260 and name CB)	(segid 3A4 and resid 311 and name CA)	17.68	0.82	0.82
	assign (segid 3A4 and resid 260 and name CB)	(segid 3A4 and resid 312 and name CA)	14.18	0.86	0.87
30	assign (segid 3A4 and resid 260 and name CB)	(segid 3A4 and resid 312 and name CB)	13.21	0.91	0.91
	assign (segid 3A4 and resid 260 and name CB)	(segid 3A4 and resid 313 and name CA)	13.45	0.67	0.67
	assign (segid 3A4 and resid 260 and name CB)	(segid 3A4 and resid 313 and name CB)	13.58	0.64	0.65
	assign (segid 3A4 and resid 260 and name CB)	(segid 3A4 and resid 314 and name CA)	16.88	0.60	0.60
	assign (segid 3A4 and resid 260 and name CB)	(segid 3A4 and resid 314 and name CB)	18.18	0.61	0.62
35	assign (segid 3A4 and resid 260 and name CB)	(segid 3A4 and resid 315 and name CA)	16.69	0.63	0.63
	assign (segid 3A4 and resid 260 and name CB)	(segid 3A4 and resid 315 and name CB)	16.86	0.73	0.72
	assign (segid 3A4 and resid 260 and name CB)	(segid 3A4 and resid 316 and name CA)	13.45	0.66	0.65
	assign (segid 3A4 and resid 260 and name CB)	(segid 3A4 and resid 317 and name CA)	13.53	0.64	0.64
	assign (segid 3A4 and resid 260 and name CB)	(segid 3A4 and resid 318 and name CA)	10.60	0.69	0.70
40	assign (segid 3A4 and resid 260 and name CB)	(segid 3A4 and resid 318 and name CB)	9.28	0.73	0.73
	assign (segid 3A4 and resid 260 and name CB)	(segid 3A4 and resid 319 and name CA)	12.66	0.57	0.58
	assign (segid 3A4 and resid 260 and name CB)	(segid 3A4 and resid 319 and name CB)	12.75	0.50	0.51
	assign (segid 3A4 and resid 260 and name CB)	(segid 3A4 and resid 347 and name CB)	17.94	0.77	0.76
	assign (segid 3A4 and resid 260 and name CB)	(segid 3A4 and resid 382 and name CA)	19.40	0.27	0.27
45	assign (segid 3A4 and resid 260 and name CB)	(segid 3A4 and resid 383 and name CA)	15.63	0.27	0.28
	assign (segid 3A4 and resid 260 and name CB)	(segid 3A4 and resid 384 and name CA)	15.71	0.22	0.22
	assign (segid 3A4 and resid 260 and name CB)	(segid 3A4 and resid 384 and name CB)	15.89	0.21	0.21
	assign (segid 3A4 and resid 260 and name CB)	(segid 3A4 and resid 385 and name CA)	18.64	0.27	0.28
	assign (segid 3A4 and resid 260 and name CB)	(segid 3A4 and resid 391 and name CA)	16.41	0.22	0.23
50	assign (segid 3A4 and resid 260 and name CB)	(segid 3A4 and resid 391 and name CB)	15.21	0.23	0.22
	assign (segid 3A4 and resid 260 and name CB)	(segid 3A4 and resid 392 and name CA)	17.40	0.32	0.33
	assign (segid 3A4 and resid 260 and name CB)	(segid 3A4 and resid 392 and name CB)	17.79	0.37	0.36
	assign (segid 3A4 and resid 260 and name CB)	(segid 3A4 and resid 393 and name CA)	14.31	0.38	0.39
	assign (segid 3A4 and resid 260 and name CB)	(segid 3A4 and resid 394 and name CA)	14.81	0.34	0.34
55	assign (segid 3A4 and resid 260 and name CB)	(segid 3A4 and resid 394 and name CB)	16.00	0.39	0.38
	assign (segid 3A4 and resid 260 and name CB)	(segid 3A4 and resid 395 and name CA)	16.34	0.37	0.37
	assign (segid 3A4 and resid 260 and name CB)	(segid 3A4 and resid 396 and name CA)	13.81	0.42	0.42
	assign (segid 3A4 and resid 260 and name CB)	(segid 3A4 and resid 396 and name CB)	13.60	0.47	0.46
	assign (segid 3A4 and resid 260 and name CB)	(segid 3A4 and resid 397 and name CA)	10.97	0.37	0.36
60	assign (segid 3A4 and resid 260 and name CB)	(segid 3A4 and resid 397 and name CB)	10.81	0.37	0.36
	assign (segid 3A4 and resid 260 and name CB)	(segid 3A4 and resid 398 and name CA)	13.40	0.41	0.41
	assign (segid 3A4 and resid 260 and name CB)	(segid 3A4 and resid 398 and name CB)	14.75	0.43	0.43
	assign (segid 3A4 and resid 260 and name CB)	(segid 3A4 and resid 399 and name CA)	14.41	0.37	0.38
	assign (segid 3A4 and resid 260 and name CB)	(segid 3A4 and resid 399 and name CB)	15.06	0.39	0.39
65	assign (segid 3A4 and resid 260 and name CB)	(segid 3A4 and resid 400 and name CA)	11.18	0.42	0.42
	assign (segid 3A4 and resid 260 and name CB)	(segid 3A4 and resid 400 and name CB)	10.05	0.47	0.47
	assign (segid 3A4 and resid 260 and name CB)	(segid 3A4 and resid 401 and name CA)	10.67	0.54	0.54
	assign (segid 3A4 and resid 260 and name CB)	(segid 3A4 and resid 402 and name CA)	14.37	0.56	0.55
	assign (segid 3A4 and resid 260 and name CB)	(segid 3A4 and resid 402 and name CB)	15.49	0.52	0.52
70	assign (segid 3A4 and resid 260 and name CB)	(segid 3A4 and resid 403 and name CA)	14.65	0.39	0.39
	assign (segid 3A4 and resid 260 and name CB)	(segid 3A4 and resid 403 and name CB)	14.56	0.36	0.37
	assign (segid 3A4 and resid 260 and name CB)	(segid 3A4 and resid 404 and name CA)	12.08	0.47	0.48
	assign (segid 3A4 and resid 260 and name CB)	(segid 3A4 and resid 404 and name CB)	10.59	0.48	0.48
	assign (segid 3A4 and resid 260 and name CB)	(segid 3A4 and resid 405 and name CA)	13.57	0.93	0.93
75	assign (segid 3A4 and resid 260 and name CB)	(segid 3A4 and resid 405 and name CB)	13.57	0.94	0.95
	assign (segid 3A4 and resid 260 and name CB)	(segid 3A4 and resid 406 and name CA)	17.01	0.81	0.80
	assign (segid 3A4 and resid 260 and name CB)	(segid 3A4 and resid 407 and name CA)	16.82	0.57	0.57
	assign (segid 3A4 and resid 260 and name CB)	(segid 3A4 and resid 407 and name CB)	16.27	0.54	0.54
	assign (segid 3A4 and resid 260 and name CB)	(segid 3A4 and resid 408 and name CA)	15.38	0.59	0.59
80	assign (segid 3A4 and resid 260 and name CB)	(segid 3A4 and resid 408 and name CB)	14.12	0.60	0.59
	assign (segid 3A4 and resid 260 and name CB)	(segid 3A4 and resid 409 and name CA)	18.02	0.70	0.71
	assign (segid 3A4 and resid 260 and name CB)	(segid 3A4 and resid 409 and name CB)	18.12	0.75	0.75
	assign (segid 3A4 and resid 260 and name CB)	(segid 3A4 and resid 424 and name CA)	16.68	1.78	1.78

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assign (segid 3A4 and resid 260 and name CB ) (segid 3A4 and resid 425 and name CA ) 15.32 1.32 1.32
assign (segid 3A4 and resid 260 and name CB ) (segid 3A4 and resid 426 and name CA ) 14.00 1.32 1.32
assign (segid 3A4 and resid 260 and name CB ) (segid 3A4 and resid 427 and name CA ) 13.01 1.26 1.27
assign (segid 3A4 and resid 260 and name CB ) (segid 3A4 and resid 428 and name CA ) 14.45 0.91 0.90
5 assign (segid 3A4 and resid 260 and name CB ) (segid 3A4 and resid 429 and name CA ) 14.66 1.05 1.06
assign (segid 3A4 and resid 260 and name CB ) (segid 3A4 and resid 430 and name CA ) 15.56 1.44 1.44
assign (segid 3A4 and resid 260 and name CB ) (segid 3A4 and resid 431 and name CA ) 14.04 0.59 0.59
assign (segid 3A4 and resid 260 and name CB ) (segid 3A4 and resid 433 and name CA ) 10.73 0.73 0.73
assign (segid 3A4 and resid 260 and name CB ) (segid 3A4 and resid 434 and name CA ) 8.67 0.73 0.73
10 assign (segid 3A4 and resid 260 and name CB ) (segid 3A4 and resid 435 and name CA ) 9.40 1.00 0.99
assign (segid 3A4 and resid 260 and name CB ) (segid 3A4 and resid 436 and name CA ) 10.25 1.83 1.84
assign (segid 3A4 and resid 260 and name CB ) (segid 3A4 and resid 437 and name CA ) 11.54 1.27 1.26
assign (segid 3A4 and resid 260 and name CB ) (segid 3A4 and resid 438 and name CA ) 12.28 0.99 0.99
assign (segid 3A4 and resid 260 and name CB ) (segid 3A4 and resid 439 and name CA ) 14.84 0.59 0.60
15 assign (segid 3A4 and resid 260 and name CB ) (segid 3A4 and resid 440 and name CA ) 16.07 0.48 0.48
assign (segid 3A4 and resid 260 and name N ) (segid 3A4 and resid 260 and name C ) 2.45 0.03 0.03
assign (segid 3A4 and resid 260 and name N ) (segid 3A4 and resid 260 and name CA ) 1.46 0.01 0.02
assign (segid 3A4 and resid 260 and name N ) (segid 3A4 and resid 260 and name CB ) 2.46 0.02 0.03
assign (segid 3A4 and resid 260 and name N ) (segid 3A4 and resid 260 and name O ) 3.48 0.03 0.02
20 assign (segid 3A4 and resid 260 and name N ) (segid 3A4 and resid 261 and name C ) 4.69 0.07 0.07
assign (segid 3A4 and resid 260 and name N ) (segid 3A4 and resid 261 and name CA ) 4.22 0.06 0.06
assign (segid 3A4 and resid 260 and name N ) (segid 3A4 and resid 261 and name N ) 2.83 0.05 0.06
assign (segid 3A4 and resid 260 and name N ) (segid 3A4 and resid 261 and name O ) 5.77 0.11 0.12
assign (segid 3A4 and resid 260 and name N ) (segid 3A4 and resid 262 and name C ) 5.67 0.07 0.07
25 assign (segid 3A4 and resid 260 and name N ) (segid 3A4 and resid 262 and name CA ) 5.30 0.09 0.09
assign (segid 3A4 and resid 260 and name N ) (segid 3A4 and resid 262 and name CB ) 5.34 0.12 0.11
assign (segid 3A4 and resid 260 and name N ) (segid 3A4 and resid 262 and name N ) 4.30 0.11 0.11
assign (segid 3A4 and resid 260 and name N ) (segid 3A4 and resid 262 and name O ) 6.89 0.08 0.08
assign (segid 3A4 and resid 260 and name N ) (segid 3A4 and resid 263 and name C ) 6.61 0.08 0.09
30 assign (segid 3A4 and resid 260 and name N ) (segid 3A4 and resid 263 and name CA ) 5.78 0.05 0.06
assign (segid 3A4 and resid 260 and name N ) (segid 3A4 and resid 263 and name CB ) 5.29 0.07 0.07
assign (segid 3A4 and resid 260 and name N ) (segid 3A4 and resid 263 and name CG ) 5.11 0.22 0.22
assign (segid 3A4 and resid 260 and name N ) (segid 3A4 and resid 263 and name N ) 4.92 0.05 0.05
assign (segid 3A4 and resid 260 and name N ) (segid 3A4 and resid 263 and name O ) 7.83 0.07 0.06
35 assign (segid 3A4 and resid 260 and name N ) (segid 3A4 and resid 264 and name CA ) 7.36 0.19 0.18
assign (segid 3A4 and resid 260 and name N ) (segid 3A4 and resid 264 and name N ) 6.23 0.15 0.14
assign (segid 3A4 and resid 260 and name N ) (segid HEM and resid 1 and name C3B) 7.62 0.13 0.12
assign (segid 3A4 and resid 260 and name N ) (segid HEM and resid 1 and name CAB) 6.63 0.12 0.11
assign (segid 3A4 and resid 260 and name N ) (segid HEM and resid 1 and name CBB) 6.39 0.26 0.25
40 assign (segid 3A4 and resid 260 and name O ) (segid 3A4 and resid 260 and name CB ) 3.32 0.07 0.08
assign (segid 3A4 and resid 260 and name O ) (segid 3A4 and resid 261 and name C ) 2.99 0.06 0.06
assign (segid 3A4 and resid 260 and name O ) (segid 3A4 and resid 261 and name CA ) 2.77 0.03 0.04
assign (segid 3A4 and resid 260 and name O ) (segid 3A4 and resid 261 and name N ) 2.25 0.02 0.02
assign (segid 3A4 and resid 260 and name O ) (segid 3A4 and resid 261 and name O ) 3.48 0.16 0.17
45 assign (segid 3A4 and resid 260 and name O ) (segid 3A4 and resid 262 and name C ) 4.14 0.18 0.18
assign (segid 3A4 and resid 260 and name O ) (segid 3A4 and resid 262 and name CA ) 4.38 0.17 0.17
assign (segid 3A4 and resid 260 and name O ) (segid 3A4 and resid 262 and name N ) 5.33 0.19 0.18
assign (segid 3A4 and resid 260 and name O ) (segid 3A4 and resid 262 and name O ) 5.09 0.21 0.22
50 assign (segid 3A4 and resid 260 and name O ) (segid 3A4 and resid 263 and name C ) 3.95 0.17 0.17
assign (segid 3A4 and resid 260 and name O ) (segid 3A4 and resid 263 and name CA ) 3.89 0.16 0.15
assign (segid 3A4 and resid 260 and name O ) (segid 3A4 and resid 263 and name CB ) 3.79 0.14 0.14
assign (segid 3A4 and resid 260 and name O ) (segid 3A4 and resid 263 and name CG ) 4.64 0.25 0.24
55 assign (segid 3A4 and resid 260 and name O ) (segid 3A4 and resid 263 and name N ) 3.38 0.15 0.14
assign (segid 3A4 and resid 260 and name O ) (segid 3A4 and resid 263 and name O ) 5.14 0.18 0.17
assign (segid 3A4 and resid 260 and name O ) (segid 3A4 and resid 264 and name C ) 5.12 0.27 0.26
assign (segid 3A4 and resid 260 and name O ) (segid 3A4 and resid 264 and name CA ) 4.00 0.24 0.23
assign (segid 3A4 and resid 260 and name O ) (segid 3A4 and resid 264 and name N ) 3.12 0.22 0.21
60 assign (segid 3A4 and resid 260 and name O ) (segid 3A4 and resid 264 and name O ) 6.26 0.26 0.27
assign (segid 3A4 and resid 260 and name O ) (segid 3A4 and resid 265 and name CA ) 6.43 0.34 0.34
assign (segid 3A4 and resid 260 and name O ) (segid 3A4 and resid 265 and name N ) 5.09 0.31 0.31
assign (segid 3A4 and resid 260 and name O ) (segid 3A4 and resid 266 and name N ) 6.91 0.32 0.32
65 assign (segid 3A4 and resid 261 and name C ) (segid 3A4 and resid 261 and name O ) 1.24 0.02 0.01
assign (segid 3A4 and resid 261 and name C ) (segid 3A4 and resid 262 and name C ) 3.06 0.07 0.06
assign (segid 3A4 and resid 261 and name C ) (segid 3A4 and resid 262 and name CA ) 2.44 0.01 0.01
assign (segid 3A4 and resid 261 and name C ) (segid 3A4 and resid 262 and name CB ) 3.72 0.02 0.01
70 assign (segid 3A4 and resid 261 and name C ) (segid 3A4 and resid 262 and name N ) 1.32 0.01 0.02
assign (segid 3A4 and resid 261 and name C ) (segid 3A4 and resid 262 and name O ) 3.90 0.10 0.09
assign (segid 3A4 and resid 261 and name C ) (segid 3A4 and resid 263 and name C ) 4.61 0.10 0.10
assign (segid 3A4 and resid 261 and name C ) (segid 3A4 and resid 263 and name CA ) 4.55 0.11 0.12
assign (segid 3A4 and resid 261 and name C ) (segid 3A4 and resid 263 and name CB ) 5.32 0.13 0.14
assign (segid 3A4 and resid 261 and name C ) (segid 3A4 and resid 263 and name CG ) 6.01 0.22 0.22
75 assign (segid 3A4 and resid 261 and name C ) (segid 3A4 and resid 263 and name N ) 3.36 0.12 0.13
assign (segid 3A4 and resid 261 and name C ) (segid 3A4 and resid 263 and name O ) 5.66 0.10 0.11
assign (segid 3A4 and resid 261 and name C ) (segid 3A4 and resid 264 and name C ) 4.86 0.09 0.09
assign (segid 3A4 and resid 261 and name C ) (segid 3A4 and resid 264 and name CA ) 4.58 0.08 0.09
assign (segid 3A4 and resid 261 and name C ) (segid 3A4 and resid 264 and name N ) 3.88 0.11 0.11
80 assign (segid 3A4 and resid 261 and name C ) (segid 3A4 and resid 264 and name O ) 6.07 0.11 0.11
assign (segid 3A4 and resid 261 and name C ) (segid 3A4 and resid 265 and name C ) 5.98 0.24 0.24
assign (segid 3A4 and resid 261 and name C ) (segid 3A4 and resid 265 and name CA ) 4.94 0.24 0.24
assign (segid 3A4 and resid 261 and name C ) (segid 3A4 and resid 265 and name N ) 4.08 0.15 0.14
assign (segid 3A4 and resid 261 and name C ) (segid 3A4 and resid 265 and name O ) 7.15 0.26 0.26
assign (segid 3A4 and resid 261 and name C ) (segid 3A4 and resid 266 and name CA ) 7.10 0.27 0.26

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	assign (segid 3A4 and resid 261 and name C) (segid 3A4 and resid 266 and name N)	5.84	0.26	0.25
	assign (segid 3A4 and resid 261 and name C) (segid 3A4 and resid 318 and name CA)	6.83	0.53	0.53
	assign (segid 3A4 and resid 261 and name C) (segid 3A4 and resid 318 and name CB)	5.64	0.55	0.54
	assign (segid 3A4 and resid 261 and name C) (segid 3A4 and resid 433 and name C)	6.46	0.37	0.36
	assign (segid 3A4 and resid 261 and name C) (segid 3A4 and resid 433 and name O)	5.50	0.39	0.40
5	assign (segid 3A4 and resid 261 and name C) (segid 3A4 and resid 434 and name C)	6.33	0.40	0.39
	assign (segid 3A4 and resid 261 and name C) (segid 3A4 and resid 434 and name CA)	5.73	0.40	0.39
	assign (segid 3A4 and resid 261 and name C) (segid 3A4 and resid 434 and name N)	6.62	0.36	0.37
	assign (segid 3A4 and resid 261 and name C) (segid 3A4 and resid 435 and name CA)	6.89	0.51	0.50
	assign (segid 3A4 and resid 261 and name C) (segid 3A4 and resid 435 and name N)	5.90	0.39	0.39
10	assign (segid 3A4 and resid 261 and name C) (segid HEM and resid 1 and name CBB)	6.93	0.30	0.29
	assign (segid 3A4 and resid 261 and name C) (segid 3A4 and resid 261 and name C)	1.52	0.00	0.01
	assign (segid 3A4 and resid 261 and name CA) (segid 3A4 and resid 261 and name O)	2.40	0.02	0.02
	assign (segid 3A4 and resid 261 and name CA) (segid 3A4 and resid 262 and name C)	4.45	0.04	0.04
	assign (segid 3A4 and resid 261 and name CA) (segid 3A4 and resid 262 and name CA)	3.83	0.02	0.01
15	assign (segid 3A4 and resid 261 and name CA) (segid 3A4 and resid 262 and name CB)	4.88	0.01	0.02
	assign (segid 3A4 and resid 261 and name CA) (segid 3A4 and resid 262 and name N)	2.45	0.02	0.02
	assign (segid 3A4 and resid 261 and name CA) (segid 3A4 and resid 262 and name O)	5.36	0.08	0.08
	assign (segid 3A4 and resid 261 and name CA) (segid 3A4 and resid 263 and name C)	5.56	0.05	0.05
	assign (segid 3A4 and resid 261 and name CA) (segid 3A4 and resid 263 and name CA)	5.55	0.07	0.08
20	assign (segid 3A4 and resid 261 and name CA) (segid 3A4 and resid 263 and name CB)	6.01	0.10	0.10
	assign (segid 3A4 and resid 261 and name CA) (segid 3A4 and resid 263 and name CG)	6.69	0.22	0.22
	assign (segid 3A4 and resid 261 and name CA) (segid 3A4 and resid 263 and name N)	4.47	0.09	0.09
	assign (segid 3A4 and resid 261 and name CA) (segid 3A4 and resid 263 and name O)	6.68	0.07	0.06
25	assign (segid 3A4 and resid 261 and name CA) (segid 3A4 and resid 264 and name C)	5.68	0.13	0.14
	assign (segid 3A4 and resid 261 and name CA) (segid 3A4 and resid 264 and name CA)	5.17	0.09	0.09
	assign (segid 3A4 and resid 261 and name CA) (segid 3A4 and resid 264 and name N)	4.62	0.05	0.06
	assign (segid 3A4 and resid 261 and name CA) (segid 3A4 and resid 264 and name O)	6.87	0.16	0.16
	assign (segid 3A4 and resid 261 and name CA) (segid 3A4 and resid 265 and name C)	7.23	0.27	0.27
	assign (segid 3A4 and resid 261 and name CA) (segid 3A4 and resid 265 and name CA)	6.06	0.28	0.27
30	assign (segid 3A4 and resid 261 and name CA) (segid 3A4 and resid 265 and name N)	5.10	0.19	0.20
	assign (segid 3A4 and resid 261 and name CA) (segid 3A4 and resid 266 and name CA)	8.48	0.26	0.26
	assign (segid 3A4 and resid 261 and name CA) (segid 3A4 and resid 266 and name N)	7.18	0.27	0.28
	assign (segid 3A4 and resid 261 and name CA) (segid 3A4 and resid 267 and name CA)	10.02	0.17	0.17
	assign (segid 3A4 and resid 261 and name CA) (segid 3A4 and resid 267 and name CB)	9.74	0.19	0.18
35	assign (segid 3A4 and resid 261 and name CA) (segid 3A4 and resid 268 and name CA)	10.60	0.17	0.17
	assign (segid 3A4 and resid 261 and name CA) (segid 3A4 and resid 268 and name CB)	9.82	0.20	0.21
	assign (segid 3A4 and resid 261 and name CA) (segid 3A4 and resid 269 and name CA)	12.25	0.33	0.33
	assign (segid 3A4 and resid 261 and name CA) (segid 3A4 and resid 270 and name CA)	14.29	0.17	0.17
	assign (segid 3A4 and resid 261 and name CA) (segid 3A4 and resid 270 and name CB)	14.05	0.14	0.14
40	assign (segid 3A4 and resid 261 and name CA) (segid 3A4 and resid 271 and name CA)	15.32	0.17	0.17
	assign (segid 3A4 and resid 261 and name CA) (segid 3A4 and resid 271 and name CB)	14.60	0.17	0.16
	assign (segid 3A4 and resid 261 and name CA) (segid 3A4 and resid 272 and name CA)	16.44	0.35	0.35
	assign (segid 3A4 and resid 261 and name CA) (segid 3A4 and resid 272 and name CB)	15.71	0.45	0.44
	assign (segid 3A4 and resid 261 and name CA) (segid 3A4 and resid 273 and name CA)	18.25	0.31	0.32
45	assign (segid 3A4 and resid 261 and name CA) (segid 3A4 and resid 273 and name CB)	17.77	0.34	0.34
	assign (segid 3A4 and resid 261 and name CA) (segid 3A4 and resid 276 and name CB)	18.19	0.23	0.24
	assign (segid 3A4 and resid 261 and name CA) (segid 3A4 and resid 277 and name CA)	18.62	0.37	0.38
	assign (segid 3A4 and resid 261 and name CA) (segid 3A4 and resid 277 and name CB)	18.40	0.45	0.45
	assign (segid 3A4 and resid 261 and name CA) (segid 3A4 and resid 280 and name CB)	18.53	0.58	0.58
50	assign (segid 3A4 and resid 261 and name CA) (segid 3A4 and resid 305 and name CA)	17.62	0.97	0.98
	assign (segid 3A4 and resid 261 and name CA) (segid 3A4 and resid 305 and name CB)	17.62	0.98	0.98
	assign (segid 3A4 and resid 261 and name CA) (segid 3A4 and resid 306 and name CA)	17.34	0.98	0.98
	assign (segid 3A4 and resid 261 and name CA) (segid 3A4 and resid 307 and name CA)	18.01	1.00	1.00
	assign (segid 3A4 and resid 261 and name CA) (segid 3A4 and resid 308 and name CA)	15.41	0.99	0.99
55	assign (segid 3A4 and resid 261 and name CA) (segid 3A4 and resid 308 and name CB)	15.47	1.00	1.00
	assign (segid 3A4 and resid 261 and name CA) (segid 3A4 and resid 309 and name CA)	12.70	0.99	0.98
	assign (segid 3A4 and resid 261 and name CA) (segid 3A4 and resid 309 and name CB)	12.89	1.04	1.04
	assign (segid 3A4 and resid 261 and name CA) (segid 3A4 and resid 310 and name CA)	14.34	0.93	0.92
	assign (segid 3A4 and resid 261 and name CA) (segid 3A4 and resid 310 and name CB)	15.81	0.92	0.92
60	assign (segid 3A4 and resid 261 and name CA) (segid 3A4 and resid 311 and name CA)	14.48	0.91	0.91
	assign (segid 3A4 and resid 261 and name CA) (segid 3A4 and resid 311 and name CB)	15.42	0.93	0.93
	assign (segid 3A4 and resid 261 and name CA) (segid 3A4 and resid 312 and name CA)	10.85	0.94	0.93
	assign (segid 3A4 and resid 261 and name CA) (segid 3A4 and resid 312 and name CB)	10.13	0.95	0.95
	assign (segid 3A4 and resid 261 and name CA) (segid 3A4 and resid 313 and name CA)	10.21	0.80	0.81
65	assign (segid 3A4 and resid 261 and name CA) (segid 3A4 and resid 313 and name CB)	10.72	0.80	0.81
	assign (segid 3A4 and resid 261 and name CA) (segid 3A4 and resid 314 and name CA)	13.27	0.71	0.70
	assign (segid 3A4 and resid 261 and name CA) (segid 3A4 and resid 314 and name CB)	14.61	0.72	0.73
	assign (segid 3A4 and resid 261 and name CA) (segid 3A4 and resid 315 and name CA)	12.63	0.68	0.67
	assign (segid 3A4 and resid 261 and name CA) (segid 3A4 and resid 315 and name CB)	12.83	0.77	0.77
70	assign (segid 3A4 and resid 261 and name CA) (segid 3A4 and resid 316 and name CA)	9.23	0.66	0.66
	assign (segid 3A4 and resid 261 and name CA) (segid 3A4 and resid 317 and name CA)	9.71	0.72	0.72
	assign (segid 3A4 and resid 261 and name CA) (segid 3A4 and resid 318 and name CA)	7.04	0.73	0.74
	assign (segid 3A4 and resid 261 and name CA) (segid 3A4 and resid 318 and name CB)	5.84	0.75	0.76
	assign (segid 3A4 and resid 261 and name CA) (segid 3A4 and resid 319 and name CA)	9.94	0.52	0.52
75	assign (segid 3A4 and resid 261 and name CA) (segid 3A4 and resid 319 and name CB)	10.39	0.41	0.42
	assign (segid 3A4 and resid 261 and name CA) (segid 3A4 and resid 346 and name CA)	17.78	0.90	0.90
	assign (segid 3A4 and resid 261 and name CA) (segid 3A4 and resid 347 and name CA)	15.84	0.82	0.83
	assign (segid 3A4 and resid 261 and name CA) (segid 3A4 and resid 347 and name CB)	14.84	0.84	0.84
	assign (segid 3A4 and resid 261 and name CA) (segid 3A4 and resid 348 and name CA)	14.46	0.96	0.95
80	assign (segid 3A4 and resid 261 and name CA) (segid 3A4 and resid 351 and name CA)	17.16	0.53	0.52
	assign (segid 3A4 and resid 261 and name CA) (segid 3A4 and resid 352 and name CA)	18.67	0.47	0.47
	assign (segid 3A4 and resid 261 and name CA) (segid 3A4 and resid 352 and name CB)	18.11	0.57	0.58

	assign (segid 3A4 and resid 261 and name CA)	(segid 3A4 and resid 361 and name CA)	18.77	0.57	0.57
	assign (segid 3A4 and resid 261 and name CA)	(segid 3A4 and resid 363 and name CA)	16.84	0.79	0.80
	assign (segid 3A4 and resid 261 and name CA)	(segid 3A4 and resid 363 and name CB)	15.86	0.70	0.70
5	assign (segid 3A4 and resid 261 and name CA)	(segid 3A4 and resid 381 and name CA)	17.60	0.61	0.61
	assign (segid 3A4 and resid 261 and name CA)	(segid 3A4 and resid 382 and name CA)	16.62	0.50	0.50
	assign (segid 3A4 and resid 261 and name CA)	(segid 3A4 and resid 382 and name CB)	17.51	0.55	0.54
	assign (segid 3A4 and resid 261 and name CA)	(segid 3A4 and resid 383 and name CA)	12.87	0.49	0.49
	assign (segid 3A4 and resid 261 and name CA)	(segid 3A4 and resid 384 and name CA)	13.90	0.35	0.35
10	assign (segid 3A4 and resid 261 and name CA)	(segid 3A4 and resid 384 and name CB)	14.33	0.31	0.31
	assign (segid 3A4 and resid 261 and name CA)	(segid 3A4 and resid 385 and name CA)	16.67	0.36	0.36
	assign (segid 3A4 and resid 261 and name CA)	(segid 3A4 and resid 390 and name CA)	18.79	0.30	0.31
	assign (segid 3A4 and resid 261 and name CA)	(segid 3A4 and resid 391 and name CA)	15.92	0.29	0.29
	assign (segid 3A4 and resid 261 and name CA)	(segid 3A4 and resid 391 and name CB)	14.56	0.29	0.29
15	assign (segid 3A4 and resid 261 and name CA)	(segid 3A4 and resid 392 and name CA)	17.77	0.27	0.27
	assign (segid 3A4 and resid 261 and name CA)	(segid 3A4 and resid 392 and name CB)	18.41	0.32	0.31
	assign (segid 3A4 and resid 261 and name CA)	(segid 3A4 and resid 393 and name CA)	15.05	0.31	0.31
	assign (segid 3A4 and resid 261 and name CA)	(segid 3A4 and resid 394 and name CA)	14.61	0.33	0.34
	assign (segid 3A4 and resid 261 and name CA)	(segid 3A4 and resid 394 and name CB)	15.49	0.39	0.40
20	assign (segid 3A4 and resid 261 and name CA)	(segid 3A4 and resid 395 and name CA)	16.67	0.36	0.36
	assign (segid 3A4 and resid 261 and name CA)	(segid 3A4 and resid 396 and name CA)	15.01	0.42	0.42
	assign (segid 3A4 and resid 261 and name CA)	(segid 3A4 and resid 396 and name CB)	15.11	0.48	0.47
	assign (segid 3A4 and resid 261 and name CA)	(segid 3A4 and resid 397 and name CA)	11.49	0.39	0.39
	assign (segid 3A4 and resid 261 and name CA)	(segid 3A4 and resid 397 and name CB)	10.93	0.40	0.40
25	assign (segid 3A4 and resid 261 and name CA)	(segid 3A4 and resid 398 and name CA)	13.19	0.43	0.43
	assign (segid 3A4 and resid 261 and name CA)	(segid 3A4 and resid 398 and name CB)	14.32	0.48	0.49
	assign (segid 3A4 and resid 261 and name CA)	(segid 3A4 and resid 399 and name CA)	15.15	0.34	0.33
	assign (segid 3A4 and resid 261 and name CA)	(segid 3A4 and resid 399 and name CB)	16.10	0.37	0.36
	assign (segid 3A4 and resid 261 and name CA)	(segid 3A4 and resid 400 and name CA)	12.52	0.45	0.45
30	assign (segid 3A4 and resid 261 and name CA)	(segid 3A4 and resid 400 and name CB)	11.65	0.54	0.55
	assign (segid 3A4 and resid 261 and name CA)	(segid 3A4 and resid 401 and name CA)	10.78	0.42	0.41
	assign (segid 3A4 and resid 261 and name CA)	(segid 3A4 and resid 402 and name CA)	14.32	0.45	0.45
	assign (segid 3A4 and resid 261 and name CA)	(segid 3A4 and resid 402 and name CB)	15.41	0.45	0.45
	assign (segid 3A4 and resid 261 and name CA)	(segid 3A4 and resid 403 and name CA)	15.62	0.32	0.32
35	assign (segid 3A4 and resid 261 and name CA)	(segid 3A4 and resid 403 and name CB)	15.90	0.36	0.36
	assign (segid 3A4 and resid 261 and name CA)	(segid 3A4 and resid 404 and name CA)	13.13	0.33	0.33
	assign (segid 3A4 and resid 261 and name CA)	(segid 3A4 and resid 404 and name CB)	11.68	0.32	0.32
	assign (segid 3A4 and resid 261 and name CA)	(segid 3A4 and resid 405 and name CA)	13.47	0.67	0.67
	assign (segid 3A4 and resid 261 and name CA)	(segid 3A4 and resid 405 and name CB)	13.04	0.75	0.76
40	assign (segid 3A4 and resid 261 and name CA)	(segid 3A4 and resid 406 and name CA)	17.15	0.65	0.65
	assign (segid 3A4 and resid 261 and name CA)	(segid 3A4 and resid 407 and name CA)	17.75	0.39	0.39
	assign (segid 3A4 and resid 261 and name CA)	(segid 3A4 and resid 407 and name CB)	17.56	0.38	0.38
	assign (segid 3A4 and resid 261 and name CA)	(segid 3A4 and resid 408 and name CA)	15.99	0.41	0.42
	assign (segid 3A4 and resid 261 and name CA)	(segid 3A4 and resid 408 and name CB)	14.57	0.42	0.41
45	assign (segid 3A4 and resid 261 and name CA)	(segid 3A4 and resid 409 and name CA)	17.86	0.49	0.49
	assign (segid 3A4 and resid 261 and name CA)	(segid 3A4 and resid 409 and name CB)	17.65	0.57	0.56
	assign (segid 3A4 and resid 261 and name CA)	(segid 3A4 and resid 414 and name CA)	18.07	0.42	0.41
	assign (segid 3A4 and resid 261 and name CA)	(segid 3A4 and resid 415 and name CA)	18.05	0.89	0.89
	assign (segid 3A4 and resid 261 and name CA)	(segid 3A4 and resid 416 and name CA)	17.14	1.14	1.15
50	assign (segid 3A4 and resid 261 and name CA)	(segid 3A4 and resid 423 and name CA)	16.50	0.87	0.87
	assign (segid 3A4 and resid 261 and name CA)	(segid 3A4 and resid 424 and name CA)	13.94	1.65	1.64
	assign (segid 3A4 and resid 261 and name CA)	(segid 3A4 and resid 425 and name CA)	12.57	0.73	0.73
	assign (segid 3A4 and resid 261 and name CA)	(segid 3A4 and resid 426 and name CA)	10.90	1.06	1.05
	assign (segid 3A4 and resid 261 and name CA)	(segid 3A4 and resid 427 and name CA)	10.14	0.74	0.74
55	assign (segid 3A4 and resid 261 and name CA)	(segid 3A4 and resid 428 and name CA)	11.79	1.10	1.09
	assign (segid 3A4 and resid 261 and name CA)	(segid 3A4 and resid 429 and name CA)	12.02	1.03	1.02
	assign (segid 3A4 and resid 261 and name CA)	(segid 3A4 and resid 430 and name CA)	13.16	1.22	1.23
	assign (segid 3A4 and resid 261 and name CA)	(segid 3A4 and resid 431 and name CA)	11.98	0.37	0.37
	assign (segid 3A4 and resid 261 and name CA)	(segid 3A4 and resid 433 and name C)	5.95	0.54	0.55
60	assign (segid 3A4 and resid 261 and name CA)	(segid 3A4 and resid 433 and name CA)	7.31	0.53	0.53
	assign (segid 3A4 and resid 261 and name CA)	(segid 3A4 and resid 433 and name O)	4.99	0.58	0.59
	assign (segid 3A4 and resid 261 and name CA)	(segid 3A4 and resid 434 and name C)	5.84	0.53	0.53
	assign (segid 3A4 and resid 261 and name CA)	(segid 3A4 and resid 434 and name CA)	5.16	0.53	0.54
	assign (segid 3A4 and resid 261 and name CA)	(segid 3A4 and resid 434 and name N)	6.09	0.52	0.53
65	assign (segid 3A4 and resid 261 and name CA)	(segid 3A4 and resid 435 and name CA)	6.52	0.65	0.64
	assign (segid 3A4 and resid 261 and name CA)	(segid 3A4 and resid 435 and name N)	5.47	0.51	0.52
	assign (segid 3A4 and resid 261 and name CA)	(segid 3A4 and resid 436 and name CA)	8.84	1.02	1.02
	assign (segid 3A4 and resid 261 and name CA)	(segid 3A4 and resid 437 and name CA)	10.63	0.83	0.84
	assign (segid 3A4 and resid 261 and name CA)	(segid 3A4 and resid 438 and name CA)	11.07	0.71	0.71
70	assign (segid 3A4 and resid 261 and name CA)	(segid 3A4 and resid 439 and name CA)	14.27	0.39	0.40
	assign (segid 3A4 and resid 261 and name CA)	(segid 3A4 and resid 440 and name CA)	15.55	0.30	0.30
	assign (segid 3A4 and resid 261 and name N)	(segid 3A4 and resid 261 and name C)	2.45	0.02	0.03
	assign (segid 3A4 and resid 261 and name N)	(segid 3A4 and resid 261 and name CA)	1.46	0.01	0.00
	assign (segid 3A4 and resid 261 and name N)	(segid 3A4 and resid 261 and name O)	3.49	0.06	0.07
75	assign (segid 3A4 and resid 261 and name N)	(segid 3A4 and resid 262 and name C)	4.76	0.04	0.04
	assign (segid 3A4 and resid 261 and name N)	(segid 3A4 and resid 262 and name CA)	4.23	0.04	0.04
	assign (segid 3A4 and resid 261 and name N)	(segid 3A4 and resid 262 and name CB)	4.98	0.06	0.05
	assign (segid 3A4 and resid 261 and name N)	(segid 3A4 and resid 262 and name N)	2.82	0.05	0.06
	assign (segid 3A4 and resid 261 and name N)	(segid 3A4 and resid 262 and name O)	5.85	0.08	0.08
80	assign (segid 3A4 and resid 261 and name N)	(segid 3A4 and resid 263 and name C)	5.74	0.07	0.06
	assign (segid 3A4 and resid 261 and name N)	(segid 3A4 and resid 263 and name CA)	5.46	0.06	0.07
	assign (segid 3A4 and resid 261 and name N)	(segid 3A4 and resid 263 and name CB)	5.57	0.09	0.09
	assign (segid 3A4 and resid 261 and name N)	(segid 3A4 and resid 263 and name CG)	6.05	0.23	0.23
	assign (segid 3A4 and resid 261 and name N)	(segid 3A4 and resid 263 and name N)	4.43	0.06	0.05

	assign (segid 3A4 and resid 261 and name N)	(segid 3A4 and resid 263 and name O)	6.94	0.08	0.07
	assign (segid 3A4 and resid 261 and name N)	(segid 3A4 and resid 264 and name C)	6.48	0.18	0.18
	assign (segid 3A4 and resid 261 and name N)	(segid 3A4 and resid 264 and name CA)	5.69	0.15	0.15
	assign (segid 3A4 and resid 261 and name N)	(segid 3A4 and resid 264 and name N)	4.92	0.10	0.09
5	assign (segid 3A4 and resid 261 and name N)	(segid 3A4 and resid 265 and name CA)	7.15	0.28	0.28
	assign (segid 3A4 and resid 261 and name N)	(segid 3A4 and resid 265 and name N)	6.06	0.22	0.22
	assign (segid 3A4 and resid 261 and name N)	(segid 3A4 and resid 318 and name CB)	6.55	0.75	0.75
	assign (segid 3A4 and resid 261 and name N)	(segid 3A4 and resid 433 and name O)	6.04	0.63	0.64
	assign (segid 3A4 and resid 261 and name N)	(segid 3A4 and resid 434 and name CA)	6.37	0.60	0.60
10	assign (segid 3A4 and resid 261 and name N)	(segid HEM and resid 1 and name CAB)	7.67	0.14	0.13
	assign (segid 3A4 and resid 261 and name N)	(segid HEM and resid 1 and name CBB)	7.14	0.29	0.30
	assign (segid 3A4 and resid 261 and name O)	(segid 3A4 and resid 262 and name C)	2.99	0.15	0.15
	assign (segid 3A4 and resid 261 and name O)	(segid 3A4 and resid 262 and name CA)	2.75	0.02	0.03
	assign (segid 3A4 and resid 261 and name O)	(segid 3A4 and resid 262 and name CB)	4.23	0.02	0.03
15	assign (segid 3A4 and resid 261 and name O)	(segid 3A4 and resid 262 and name N)	2.23	0.01	0.02
	assign (segid 3A4 and resid 261 and name O)	(segid 3A4 and resid 262 and name O)	3.48	0.18	0.18
	assign (segid 3A4 and resid 261 and name O)	(segid 3A4 and resid 263 and name C)	4.16	0.27	0.27
	assign (segid 3A4 and resid 261 and name O)	(segid 3A4 and resid 263 and name CA)	4.45	0.26	0.26
	assign (segid 3A4 and resid 261 and name O)	(segid 3A4 and resid 263 and name CB)	5.45	0.28	0.27
20	assign (segid 3A4 and resid 261 and name O)	(segid 3A4 and resid 263 and name CG)	6.34	0.31	0.31
	assign (segid 3A4 and resid 261 and name O)	(segid 3A4 and resid 263 and name N)	3.49	0.22	0.23
	assign (segid 3A4 and resid 261 and name O)	(segid 3A4 and resid 263 and name O)	5.05	0.26	0.27
	assign (segid 3A4 and resid 261 and name O)	(segid 3A4 and resid 264 and name C)	3.83	0.16	0.17
	assign (segid 3A4 and resid 261 and name O)	(segid 3A4 and resid 264 and name CA)	3.82	0.25	0.25
25	assign (segid 3A4 and resid 261 and name O)	(segid 3A4 and resid 264 and name N)	3.37	0.29	0.30
	assign (segid 3A4 and resid 261 and name O)	(segid 3A4 and resid 264 and name O)	5.00	0.13	0.14
	assign (segid 3A4 and resid 261 and name O)	(segid 3A4 and resid 265 and name C)	4.89	0.25	0.26
	assign (segid 3A4 and resid 261 and name O)	(segid 3A4 and resid 265 and name CA)	3.78	0.23	0.24
	assign (segid 3A4 and resid 261 and name O)	(segid 3A4 and resid 265 and name N)	2.96	0.17	0.17
30	assign (segid 3A4 and resid 261 and name O)	(segid 3A4 and resid 265 and name O)	6.04	0.27	0.26
	assign (segid 3A4 and resid 261 and name O)	(segid 3A4 and resid 266 and name C)	7.16	0.30	0.29
	assign (segid 3A4 and resid 261 and name O)	(segid 3A4 and resid 266 and name CA)	6.24	0.32	0.32
	assign (segid 3A4 and resid 261 and name O)	(segid 3A4 and resid 266 and name N)	4.90	0.31	0.31
	assign (segid 3A4 and resid 261 and name O)	(segid 3A4 and resid 267 and name N)	6.91	0.31	0.31
35	assign (segid 3A4 and resid 261 and name O)	(segid 3A4 and resid 316 and name O)	7.00	0.56	0.56
	assign (segid 3A4 and resid 261 and name O)	(segid 3A4 and resid 318 and name CA)	7.17	0.37	0.37
	assign (segid 3A4 and resid 261 and name O)	(segid 3A4 and resid 318 and name CB)	6.12	0.35	0.34
	assign (segid 3A4 and resid 261 and name O)	(segid 3A4 and resid 433 and name C)	6.49	0.33	0.33
	assign (segid 3A4 and resid 261 and name O)	(segid 3A4 and resid 433 and name O)	5.67	0.39	0.40
40	assign (segid 3A4 and resid 261 and name O)	(segid 3A4 and resid 434 and name C)	5.91	0.25	0.25
	assign (segid 3A4 and resid 261 and name O)	(segid 3A4 and resid 434 and name CA)	5.52	0.25	0.26
	assign (segid 3A4 and resid 261 and name O)	(segid 3A4 and resid 434 and name N)	6.50	0.27	0.27
	assign (segid 3A4 and resid 261 and name O)	(segid 3A4 and resid 434 and name O)	6.96	0.33	0.33
	assign (segid 3A4 and resid 261 and name O)	(segid 3A4 and resid 435 and name C)	6.97	0.58	0.59
45	assign (segid 3A4 and resid 261 and name O)	(segid 3A4 and resid 435 and name CA)	6.22	0.45	0.45
	assign (segid 3A4 and resid 261 and name O)	(segid 3A4 and resid 435 and name N)	5.36	0.30	0.31
	assign (segid 3A4 and resid 261 and name O)	(segid 3A4 and resid 435 and name O)	6.67	0.76	0.75
	assign (segid 3A4 and resid 262 and name C)	(segid 3A4 and resid 262 and name CB)	2.49	0.04	0.03
	assign (segid 3A4 and resid 262 and name C)	(segid 3A4 and resid 262 and name O)	1.24	0.01	0.00
50	assign (segid 3A4 and resid 262 and name C)	(segid 3A4 and resid 263 and name C)	3.02	0.05	0.05
	assign (segid 3A4 and resid 262 and name C)	(segid 3A4 and resid 263 and name CA)	2.44	0.02	0.01
	assign (segid 3A4 and resid 262 and name C)	(segid 3A4 and resid 263 and name CB)	3.71	0.03	0.04
	assign (segid 3A4 and resid 262 and name C)	(segid 3A4 and resid 263 and name CG)	4.22	0.13	0.14
	assign (segid 3A4 and resid 262 and name C)	(segid 3A4 and resid 263 and name N)	1.32	0.01	0.02
55	assign (segid 3A4 and resid 262 and name C)	(segid 3A4 and resid 263 and name O)	3.84	0.06	0.07
	assign (segid 3A4 and resid 262 and name C)	(segid 3A4 and resid 264 and name C)	4.54	0.10	0.10
	assign (segid 3A4 and resid 262 and name C)	(segid 3A4 and resid 264 and name CA)	4.47	0.09	0.08
	assign (segid 3A4 and resid 262 and name C)	(segid 3A4 and resid 264 and name N)	3.29	0.11	0.10
	assign (segid 3A4 and resid 262 and name C)	(segid 3A4 and resid 264 and name O)	5.60	0.08	0.09
60	assign (segid 3A4 and resid 262 and name C)	(segid 3A4 and resid 265 and name C)	4.77	0.13	0.14
	assign (segid 3A4 and resid 262 and name C)	(segid 3A4 and resid 265 and name CA)	4.53	0.17	0.17
	assign (segid 3A4 and resid 262 and name C)	(segid 3A4 and resid 265 and name N)	3.82	0.15	0.14
	assign (segid 3A4 and resid 262 and name C)	(segid 3A4 and resid 265 and name O)	5.98	0.15	0.15
	assign (segid 3A4 and resid 262 and name C)	(segid 3A4 and resid 266 and name C)	6.00	0.14	0.15
65	assign (segid 3A4 and resid 262 and name C)	(segid 3A4 and resid 266 and name CA)	4.86	0.16	0.17
	assign (segid 3A4 and resid 262 and name C)	(segid 3A4 and resid 266 and name N)	4.00	0.13	0.13
	assign (segid 3A4 and resid 262 and name C)	(segid 3A4 and resid 266 and name O)	7.13	0.15	0.16
	assign (segid 3A4 and resid 262 and name C)	(segid 3A4 and resid 267 and name CA)	7.28	0.15	0.15
	assign (segid 3A4 and resid 262 and name C)	(segid 3A4 and resid 267 and name CB)	7.38	0.17	0.17
70	assign (segid 3A4 and resid 262 and name C)	(segid 3A4 and resid 267 and name N)	5.95	0.14	0.15
	assign (segid 3A4 and resid 262 and name C)	(segid 3A4 and resid 268 and name N)	7.82	0.07	0.07
	assign (segid 3A4 and resid 262 and name C)	(segid 3A4 and resid 312 and name C)	7.19	0.74	0.74
	assign (segid 3A4 and resid 262 and name C)	(segid 3A4 and resid 312 and name CB)	6.37	0.85	0.85
	assign (segid 3A4 and resid 262 and name C)	(segid 3A4 and resid 312 and name O)	7.10	0.68	0.69
75	assign (segid 3A4 and resid 262 and name C)	(segid 3A4 and resid 318 and name CB)	7.18	0.37	0.36
	assign (segid 3A4 and resid 262 and name C)	(segid 3A4 and resid 401 and name CA)	7.31	0.49	0.48
	assign (segid 3A4 and resid 262 and name C)	(segid HEM and resid 1 and name CAB)	7.68	0.10	0.11
	assign (segid 3A4 and resid 262 and name C)	(segid HEM and resid 1 and name CBB)	6.54	0.13	0.12
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 262 and name C)	1.53	0.02	0.01
80	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 262 and name CB)	1.53	0.02	0.01
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 262 and name O)	2.39	0.02	0.02
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 263 and name C)	4.41	0.03	0.04
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 263 and name CA)	3.82	0.01	0.01

	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 263 and name CB)	4.87	0.02	0.02
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 263 and name CG)	5.18	0.13	0.13
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 263 and name N)	2.44	0.03	0.02
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 263 and name O)	5.30	0.05	0.06
5	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 264 and name C)	5.47	0.12	0.12
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 264 and name CA)	5.44	0.10	0.11
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 264 and name N)	4.38	0.11	0.11
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 264 and name O)	6.59	0.12	0.12
10	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 265 and name C)	5.57	0.17	0.18
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 265 and name CA)	5.06	0.22	0.22
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 265 and name N)	4.52	0.16	0.17
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 265 and name O)	6.75	0.20	0.19
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 266 and name C)	7.23	0.15	0.16
15	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 266 and name CA)	5.98	0.19	0.19
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 266 and name N)	5.02	0.15	0.16
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 267 and name CA)	8.63	0.12	0.12
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 267 and name CB)	8.78	0.13	0.13
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 267 and name N)	7.29	0.13	0.12
20	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 268 and name CA)	9.88	0.07	0.06
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 268 and name CB)	9.44	0.11	0.11
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 269 and name CA)	10.48	0.25	0.24
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 270 and name CA)	12.22	0.15	0.15
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 270 and name CB)	11.87	0.17	0.17
25	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 271 and name CA)	14.10	0.13	0.13
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 271 and name CB)	13.72	0.10	0.11
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 272 and name CA)	15.20	0.31	0.30
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 272 and name CB)	14.55	0.43	0.43
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 273 and name CA)	16.29	0.26	0.25
30	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 273 and name CB)	15.60	0.24	0.24
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 274 and name CA)	18.32	0.51	0.51
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 276 and name CA)	16.61	0.23	0.24
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 276 and name CB)	15.40	0.21	0.20
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 277 and name CA)	16.08	0.38	0.38
35	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 277 and name CB)	16.11	0.47	0.47
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 279 and name CB)	19.26	0.42	0.42
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 280 and name CA)	16.90	0.58	0.58
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 280 and name CB)	15.45	0.57	0.57
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 304 and name CA)	17.19	0.93	0.92
40	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 304 and name CB)	17.69	0.87	0.88
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 305 and name CA)	14.07	0.97	0.98
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 305 and name CB)	14.18	0.98	0.98
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 306 and name CA)	13.61	1.01	1.01
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 307 and name CA)	14.23	1.00	1.00
45	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 307 and name CB)	15.54	0.99	0.98
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 308 and name CA)	11.75	0.95	0.96
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 308 and name CB)	11.91	0.95	0.96
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 309 and name CA)	8.92	0.99	0.99
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 309 and name CB)	9.15	1.08	1.07
50	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 310 and name CA)	10.65	0.88	0.88
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 310 and name CB)	12.12	0.88	0.88
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 311 and name CA)	11.01	0.84	0.85
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 311 and name CB)	11.96	0.86	0.87
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 312 and name CA)	7.51	0.85	0.85
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 312 and name CB)	6.67	0.87	0.88
55	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 312 and name O)	6.73	0.74	0.74
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 313 and name CA)	7.05	0.69	0.70
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 313 and name CB)	7.48	0.67	0.67
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 313 and name CG)	6.62	0.66	0.67
60	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 314 and name CA)	10.45	0.63	0.63
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 314 and name CB)	11.65	0.65	0.66
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 315 and name CA)	10.28	0.64	0.65
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 315 and name CB)	10.39	0.68	0.68
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 316 and name CA)	7.58	0.78	0.79
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 317 and name CA)	8.29	0.61	0.60
65	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 318 and name CA)	6.95	0.31	0.31
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 318 and name CB)	5.73	0.36	0.37
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 318 and name N)	7.02	0.44	0.44
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 319 and name CA)	10.14	0.36	0.36
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 319 and name CB)	10.39	0.39	0.39
70	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 346 and name CA)	17.39	0.82	0.83
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 346 and name CB)	18.02	0.99	0.98
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 347 and name CA)	14.82	0.73	0.72
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 347 and name CB)	13.81	0.70	0.71
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 348 and name CA)	13.48	0.92	0.91
75	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 349 and name CA)	17.07	0.94	0.94
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 350 and name CA)	17.61	0.58	0.58
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 350 and name CB)	17.49	0.60	0.60
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 351 and name CA)	15.05	0.43	0.44
80	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 352 and name CA)	16.82	0.60	0.60
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 352 and name CB)	16.52	0.73	0.73
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 357 and name CB)	18.57	0.43	0.44
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 360 and name CA)	17.94	0.60	0.59
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 360 and name CB)	18.36	0.64	0.63

	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 361 and name CA)	16.93	0.66	0.65
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 361 and name CB)	17.83	0.73	0.72
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 362 and name CA)	17.00	0.61	0.62
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 362 and name CB)	18.31	0.68	0.67
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 363 and name CA)	14.21	0.69	0.69
5	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 363 and name CB)	13.34	0.59	0.59
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 364 and name CA)	16.15	0.78	0.79
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 364 and name CB)	17.45	0.78	0.77
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 365 and name CA)	15.17	0.97	0.98
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 365 and name CB)	14.96	0.99	1.00
10	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 381 and name CA)	14.86	0.57	0.56
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 382 and name CA)	14.45	0.35	0.36
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 382 and name CB)	15.55	0.37	0.38
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 383 and name CA)	10.78	0.34	0.35
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 384 and name CA)	12.02	0.29	0.28
15	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 384 and name CB)	12.22	0.28	0.28
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 385 and name CA)	15.20	0.29	0.29
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 386 and name CA)	18.62	0.26	0.26
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 390 and name CA)	17.38	0.23	0.24
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 390 and name CB)	17.84	0.33	0.33
20	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 391 and name CA)	14.64	0.21	0.21
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 391 and name CB)	13.17	0.23	0.22
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 392 and name CA)	16.56	0.19	0.19
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 392 and name CB)	17.47	0.21	0.20
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 393 and name CA)	13.75	0.24	0.24
25	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 394 and name CA)	12.46	0.33	0.33
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 394 and name CB)	13.22	0.40	0.41
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 395 and name CA)	14.26	0.43	0.42
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 396 and name CA)	13.12	0.45	0.45
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 396 and name CB)	13.58	0.49	0.48
30	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 397 and name CA)	9.38	0.45	0.44
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 397 and name CB)	8.85	0.42	0.43
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 398 and name CA)	10.19	0.51	0.51
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 398 and name CB)	11.21	0.57	0.56
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 399 and name CA)	12.49	0.45	0.44
35	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 399 and name CB)	13.63	0.46	0.46
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 400 and name CA)	10.43	0.58	0.58
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 400 and name CB)	9.89	0.67	0.68
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 401 and name CA)	7.94	0.54	0.54
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 402 and name CA)	11.20	0.55	0.55
40	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 402 and name CB)	12.20	0.55	0.56
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 403 and name CA)	13.15	0.48	0.48
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 403 and name CB)	13.63	0.51	0.51
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 404 and name CA)	11.15	0.49	0.49
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 404 and name CB)	9.85	0.49	0.48
45	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 405 and name CA)	10.92	0.72	0.72
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 405 and name CB)	10.20	0.80	0.80
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 406 and name CA)	14.48	0.77	0.77
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 407 and name CA)	15.75	0.54	0.54
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 407 and name CB)	15.73	0.53	0.53
50	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 408 and name CA)	14.38	0.49	0.49
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 408 and name CB)	13.02	0.48	0.48
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 409 and name CA)	15.81	0.56	0.57
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 409 and name CB)	15.36	0.64	0.65
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 412 and name CA)	18.83	0.24	0.25
55	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 414 and name CA)	17.26	0.45	0.46
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 415 and name CA)	17.70	0.74	0.74
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 416 and name CA)	17.38	1.10	1.10
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 423 and name CA)	17.71	1.10	1.10
60	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 424 and name CA)	15.16	1.72	1.72
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 425 and name CA)	14.28	0.51	0.50
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 426 and name CA)	12.93	0.95	0.95
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 427 and name CA)	12.62	0.58	0.57
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 428 and name CA)	14.41	1.26	1.25
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 429 and name CA)	14.49	1.02	1.01
65	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 430 and name CA)	15.38	1.06	1.07
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 431 and name CA)	13.93	0.38	0.39
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 433 and name CA)	9.21	0.42	0.41
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 433 and name O)	7.06	0.38	0.38
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 434 and name CA)	7.69	0.38	0.38
70	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 435 and name CA)	8.87	0.46	0.47
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 436 and name CA)	11.79	0.63	0.62
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 437 and name CA)	13.20	0.72	0.72
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 438 and name CA)	12.71	0.55	0.55
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 439 and name CA)	15.69	0.27	0.28
75	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 440 and name CA)	16.15	0.17	0.17
	assign (segid 3A4 and resid 262 and name CA)	(segid HEM and resid 1 and name C3B)	7.67	0.10	0.10
	assign (segid 3A4 and resid 262 and name CA)	(segid HEM and resid 1 and name CBB)	6.60	0.12	0.11
	assign (segid 3A4 and resid 262 and name CA)	(segid HEM and resid 1 and name CMB)	5.47	0.19	0.20
80	assign (segid 3A4 and resid 262 and name CA)	(segid HEM and resid 1 and name CMB)	7.38	0.17	0.17
	assign (segid 3A4 and resid 262 and name CA)	(segid 3A4 and resid 263 and name C)	5.41	0.04	0.04
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 263 and name CA)	4.46	0.06	0.05
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 263 and name CB)	5.31	0.08	0.08

	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 263 and name CG)	5.18	0.14	0.13
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 263 and name N)	3.12	0.06	0.06
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 263 and name O)	6.26	0.04	0.04
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 264 and name C)	6.87	0.12	0.12
5	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 264 and name CA)	6.80	0.10	0.09
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 264 and name N)	5.60	0.09	0.08
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 265 and name C)	6.73	0.18	0.18
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 265 and name CA)	6.41	0.24	0.24
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 265 and name N)	5.96	0.17	0.17
10	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 266 and name CA)	6.74	0.13	0.14
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 266 and name N)	6.02	0.12	0.13
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 267 and name CA)	9.62	0.14	0.14
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 267 and name CB)	9.81	0.17	0.17
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 268 and name CA)	11.12	0.07	0.07
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 268 and name CB)	10.78	0.13	0.12
15	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 269 and name CA)	11.41	0.24	0.24
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 270 and name CA)	12.97	0.15	0.14
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 270 and name CB)	12.54	0.18	0.19
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 271 and name CA)	15.13	0.12	0.12
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 271 and name CB)	14.84	0.10	0.11
20	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 272 and name CA)	16.84	0.30	0.30
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 272 and name CB)	15.62	0.45	0.44
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 273 and name CA)	17.06	0.25	0.24
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 273 and name CB)	16.29	0.20	0.21
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 274 and name CA)	19.03	0.51	0.50
25	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 276 and name CA)	16.93	0.21	0.22
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 276 and name CB)	15.75	0.21	0.20
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 277 and name CA)	16.49	0.36	0.36
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 277 and name CB)	16.64	0.46	0.45
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 279 and name CB)	19.31	0.39	0.38
30	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 280 and name CA)	16.85	0.55	0.54
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 280 and name CB)	15.44	0.52	0.51
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 304 and name CA)	16.66	0.88	0.87
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 304 and name CB)	17.27	0.82	0.82
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 305 and name CA)	13.52	0.92	0.92
35	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 305 and name CB)	13.62	0.95	0.94
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 306 and name CA)	12.72	0.98	0.98
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 307 and name CA)	13.52	0.93	0.93
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 307 and name CB)	14.89	0.91	0.92
40	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 308 and name CA)	11.38	0.87	0.86
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 308 and name CB)	11.63	0.85	0.86
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 309 and name CA)	8.21	0.91	0.92
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 309 and name CB)	8.27	1.02	1.02
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 310 and name CA)	9.79	0.82	0.81
45	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 310 and name CB)	11.21	0.82	0.83
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 311 and name CA)	10.63	0.77	0.76
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 311 and name CB)	11.68	0.78	0.78
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 312 and name C)	6.75	0.75	0.75
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 312 and name CA)	7.42	0.76	0.76
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 312 and name CB)	6.61	0.77	0.78
50	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 312 and name O)	6.71	0.73	0.73
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 313 and name CA)	6.44	0.69	0.70
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 313 and name CB)	6.59	0.66	0.66
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 313 and name CG)	5.57	0.62	0.62
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 313 and name N)	6.61	0.76	0.77
55	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 314 and name CA)	10.05	0.66	0.66
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 314 and name CB)	11.23	0.65	0.65
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 315 and name CA)	10.43	0.68	0.68
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 315 and name CB)	10.64	0.66	0.67
60	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 316 and name CA)	7.98	0.87	0.88
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 317 and name CA)	8.19	0.62	0.61
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 318 and name CA)	7.04	0.27	0.28
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 318 and name CB)	5.79	0.29	0.30
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 318 and name N)	6.99	0.39	0.39
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 319 and name CA)	9.90	0.41	0.41
65	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 319 and name CB)	9.95	0.47	0.47
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 346 and name CA)	17.18	0.82	0.83
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 346 and name CB)	17.90	0.98	0.99
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 347 and name CA)	14.41	0.73	0.73
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 347 and name CB)	13.33	0.69	0.68
70	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 348 and name CA)	13.40	0.92	0.93
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 349 and name CA)	17.01	0.94	0.94
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 349 and name CB)	18.18	0.92	0.93
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 350 and name CA)	17.25	0.64	0.63
75	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 350 and name CB)	17.02	0.65	0.64
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 351 and name CA)	14.72	0.52	0.52
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 352 and name CB)	16.78	0.71	0.72
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 357 and name CB)	18.29	0.50	0.51
80	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 360 and name CA)	18.02	0.65	0.66
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 360 and name CB)	18.41	0.72	0.73
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 361 and name CA)	17.32	0.70	0.71
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 361 and name CB)	18.31	0.78	0.78

	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 362 and name CA)	17.38	0.62	0.62
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 362 and name CB)	18.63	0.66	0.67
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 363 and name CA)	14.54	0.65	0.64
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 363 and name CB)	13.77	0.55	0.56
5	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 364 and name CA)	16.20	0.71	0.72
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 364 and name CB)	17.48	0.71	0.71
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 365 and name CA)	14.97	0.88	0.88
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 365 and name CB)	14.79	0.89	0.90
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 381 and name CA)	14.02	0.57	0.58
10	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 382 and name CA)	13.56	0.34	0.34
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 382 and name CB)	14.72	0.34	0.35
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 383 and name CA)	9.89	0.34	0.34
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 384 and name CA)	10.84	0.29	0.28
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 384 and name CB)	10.93	0.26	0.26
15	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 385 and name CA)	14.17	0.30	0.29
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 386 and name CA)	17.51	0.28	0.28
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 389 and name CA)	18.93	0.31	0.31
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 389 and name CB)	19.10	0.48	0.48
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 390 and name CA)	16.14	0.21	0.21
20	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 390 and name CB)	16.55	0.29	0.29
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 391 and name CA)	13.36	0.17	0.17
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 391 and name CB)	11.87	0.19	0.18
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 392 and name CA)	15.20	0.16	0.17
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 392 and name CB)	16.16	0.18	0.18
25	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 393 and name CA)	12.38	0.24	0.24
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 394 and name CA)	10.97	0.31	0.32
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 394 and name CB)	11.74	0.39	0.39
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 395 and name CA)	12.76	0.43	0.43
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 396 and name CA)	11.75	0.50	0.49
30	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 396 and name CB)	12.25	0.52	0.52
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 397 and name CA)	7.97	0.47	0.48
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 397 and name CB)	7.41	0.43	0.43
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 397 and name O)	7.12	0.57	0.57
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 398 and name CA)	8.79	0.53	0.52
35	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 398 and name CB)	9.78	0.56	0.56
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 399 and name CA)	11.25	0.50	0.49
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 399 and name CB)	12.37	0.52	0.52
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 400 and name CA)	9.44	0.64	0.64
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 400 and name CB)	8.90	0.72	0.73
40	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 401 and name CA)	7.06	0.59	0.59
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 402 and name CA)	10.36	0.57	0.57
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 402 and name CB)	11.23	0.57	0.58
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 403 and name CA)	12.46	0.53	0.52
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 403 and name CB)	12.87	0.56	0.56
45	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 404 and name CA)	10.84	0.52	0.51
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 404 and name CB)	9.58	0.50	0.50
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 405 and name CA)	10.78	0.71	0.71
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 405 and name CB)	10.01	0.77	0.77
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 406 and name CA)	14.17	0.78	0.77
50	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 407 and name CA)	15.60	0.56	0.57
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 407 and name CB)	15.51	0.56	0.56
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 408 and name CA)	14.60	0.49	0.49
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 408 and name CB)	13.32	0.48	0.48
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 409 and name CA)	16.06	0.58	0.58
55	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 409 and name CB)	15.57	0.67	0.67
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 412 and name CA)	19.35	0.25	0.26
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 414 and name CA)	18.19	0.47	0.47
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 424 and name CA)	16.61	1.78	1.78
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 425 and name CA)	15.68	0.59	0.59
60	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 426 and name CA)	14.26	1.05	1.05
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 427 and name CA)	13.80	0.50	0.50
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 428 and name CA)	15.44	1.24	1.24
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 429 and name CA)	15.30	1.01	1.01
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 430 and name CA)	15.92	1.06	1.07
65	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 431 and name CA)	14.19	0.48	0.49
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 433 and name CA)	9.98	0.42	0.42
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 434 and name CA)	8.86	0.39	0.38
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 435 and name CA)	10.30	0.48	0.48
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 436 and name CA)	13.15	0.67	0.66
70	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 437 and name CA)	14.64	0.72	0.71
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 438 and name CA)	14.16	0.55	0.55
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 439 and name CA)	17.08	0.27	0.26
	assign (segid 3A4 and resid 262 and name CB)	(segid 3A4 and resid 440 and name CA)	17.39	0.15	0.16
	assign (segid 3A4 and resid 262 and name CB)	(segid HEM and resid 1 and name C2B)	6.87	0.11	0.11
75	assign (segid 3A4 and resid 262 and name CB)	(segid HEM and resid 1 and name C3B)	6.47	0.07	0.06
	assign (segid 3A4 and resid 262 and name CB)	(segid HEM and resid 1 and name C4B)	7.73	0.05	0.04
	assign (segid 3A4 and resid 262 and name CB)	(segid HEM and resid 1 and name CAB)	5.32	0.09	0.09
	assign (segid 3A4 and resid 262 and name CB)	(segid HEM and resid 1 and name CBB)	4.14	0.13	0.12
	assign (segid 3A4 and resid 262 and name CB)	(segid HEM and resid 1 and name CMB)	6.34	0.17	0.17
80	assign (segid 3A4 and resid 262 and name N)	(segid 3A4 and resid 262 and name C)	2.47	0.02	0.02
	assign (segid 3A4 and resid 262 and name N)	(segid 3A4 and resid 262 and name CA)	1.46	0.01	0.01
	assign (segid 3A4 and resid 262 and name N)	(segid 3A4 and resid 262 and name CB)	2.46	0.02	0.03
	assign (segid 3A4 and resid 262 and name N)	(segid 3A4 and resid 262 and name O)	3.51	0.04	0.03

	assign (segid 3A4 and resid 262 and name N)	(segid 3A4 and resid 263 and name C)	4.72	0.05	0.05
	assign (segid 3A4 and resid 262 and name N)	(segid 3A4 and resid 263 and name CA)	4.26	0.04	0.04
	assign (segid 3A4 and resid 262 and name N)	(segid 3A4 and resid 263 and name CB)	5.03	0.05	0.04
	assign (segid 3A4 and resid 262 and name N)	(segid 3A4 and resid 263 and name CG)	5.42	0.15	0.14
5	assign (segid 3A4 and resid 262 and name N)	(segid 3A4 and resid 263 and name N)	2.85	0.05	0.05
	assign (segid 3A4 and resid 262 and name N)	(segid 3A4 and resid 263 and name O)	5.79	0.06	0.06
	assign (segid 3A4 and resid 262 and name N)	(segid 3A4 and resid 264 and name C)	5.58	0.11	0.12
	assign (segid 3A4 and resid 262 and name N)	(segid 3A4 and resid 264 and name CA)	5.31	0.10	0.11
	assign (segid 3A4 and resid 262 and name N)	(segid 3A4 and resid 264 and name N)	4.32	0.09	0.09
10	assign (segid 3A4 and resid 262 and name N)	(segid 3A4 and resid 264 and name O)	6.79	0.12	0.12
	assign (segid 3A4 and resid 262 and name N)	(segid 3A4 and resid 265 and name C)	6.30	0.18	0.19
	assign (segid 3A4 and resid 262 and name N)	(segid 3A4 and resid 265 and name CA)	5.50	0.20	0.20
	assign (segid 3A4 and resid 262 and name N)	(segid 3A4 and resid 265 and name N)	4.74	0.14	0.14
	assign (segid 3A4 and resid 262 and name N)	(segid 3A4 and resid 265 and name O)	7.50	0.21	0.21
15	assign (segid 3A4 and resid 262 and name N)	(segid 3A4 and resid 266 and name CA)	7.04	0.21	0.21
	assign (segid 3A4 and resid 262 and name N)	(segid 3A4 and resid 266 and name N)	5.93	0.19	0.19
	assign (segid 3A4 and resid 262 and name N)	(segid 3A4 and resid 318 and name CA)	6.69	0.51	0.51
	assign (segid 3A4 and resid 262 and name N)	(segid 3A4 and resid 318 and name CB)	5.39	0.55	0.55
	assign (segid 3A4 and resid 262 and name N)	(segid 3A4 and resid 433 and name O)	6.18	0.41	0.41
20	assign (segid 3A4 and resid 262 and name N)	(segid 3A4 and resid 434 and name CA)	6.78	0.44	0.45
	assign (segid 3A4 and resid 262 and name N)	(segid 3A4 and resid 435 and name N)	7.15	0.42	0.42
	assign (segid 3A4 and resid 262 and name N)	(segid HEM and resid 1 and name C3B)	7.61	0.16	0.16
	assign (segid 3A4 and resid 262 and name N)	(segid HEM and resid 1 and name CAB)	6.62	0.17	0.17
	assign (segid 3A4 and resid 262 and name N)	(segid HEM and resid 1 and name CBB)	5.70	0.26	0.26
25	assign (segid 3A4 and resid 262 and name N)	(segid HEM and resid 1 and name CMB)	7.49	0.27	0.27
	assign (segid 3A4 and resid 262 and name O)	(segid 3A4 and resid 262 and name CB)	3.26	0.07	0.07
	assign (segid 3A4 and resid 262 and name O)	(segid 3A4 and resid 263 and name C)	3.01	0.06	0.05
	assign (segid 3A4 and resid 262 and name O)	(segid 3A4 and resid 263 and name CA)	2.78	0.02	0.02
	assign (segid 3A4 and resid 262 and name O)	(segid 3A4 and resid 263 and name CB)	4.26	0.04	0.04
30	assign (segid 3A4 and resid 262 and name O)	(segid 3A4 and resid 263 and name CG)	4.88	0.14	0.13
	assign (segid 3A4 and resid 262 and name O)	(segid 3A4 and resid 263 and name N)	2.25	0.00	0.01
	assign (segid 3A4 and resid 262 and name O)	(segid 3A4 and resid 263 and name O)	3.46	0.08	0.07
	assign (segid 3A4 and resid 262 and name O)	(segid 3A4 and resid 264 and name C)	4.16	0.14	0.14
	assign (segid 3A4 and resid 262 and name O)	(segid 3A4 and resid 264 and name CA)	4.44	0.13	0.12
35	assign (segid 3A4 and resid 262 and name O)	(segid 3A4 and resid 264 and name N)	3.49	0.13	0.12
	assign (segid 3A4 and resid 262 and name O)	(segid 3A4 and resid 265 and name C)	5.06	0.13	0.13
	assign (segid 3A4 and resid 262 and name O)	(segid 3A4 and resid 265 and name CA)	3.77	0.16	0.15
	assign (segid 3A4 and resid 262 and name O)	(segid 3A4 and resid 265 and name N)	3.82	0.20	0.19
	assign (segid 3A4 and resid 262 and name O)	(segid 3A4 and resid 265 and name O)	3.39	0.19	0.18
40	assign (segid 3A4 and resid 262 and name O)	(segid 3A4 and resid 265 and name N)	4.92	0.16	0.16
	assign (segid 3A4 and resid 262 and name O)	(segid 3A4 and resid 266 and name C)	4.91	0.17	0.17
	assign (segid 3A4 and resid 262 and name O)	(segid 3A4 and resid 266 and name CA)	3.68	0.18	0.18
	assign (segid 3A4 and resid 262 and name O)	(segid 3A4 and resid 266 and name N)	2.89	0.14	0.13
	assign (segid 3A4 and resid 262 and name O)	(segid 3A4 and resid 266 and name O)	6.00	0.18	0.17
45	assign (segid 3A4 and resid 262 and name O)	(segid 3A4 and resid 267 and name C)	7.24	0.14	0.14
	assign (segid 3A4 and resid 262 and name O)	(segid 3A4 and resid 267 and name CA)	6.41	0.17	0.18
	assign (segid 3A4 and resid 262 and name O)	(segid 3A4 and resid 267 and name CB)	6.73	0.17	0.18
	assign (segid 3A4 and resid 262 and name O)	(segid 3A4 and resid 267 and name N)	5.02	0.16	0.17
	assign (segid 3A4 and resid 262 and name O)	(segid 3A4 and resid 268 and name N)	6.93	0.12	0.12
50	assign (segid 3A4 and resid 262 and name O)	(segid 3A4 and resid 269 and name N)	7.74	0.14	0.14
	assign (segid 3A4 and resid 262 and name O)	(segid 3A4 and resid 312 and name C)	6.48	0.74	0.73
	assign (segid 3A4 and resid 262 and name O)	(segid 3A4 and resid 312 and name CA)	6.54	0.84	0.85
	assign (segid 3A4 and resid 262 and name O)	(segid 3A4 and resid 312 and name CB)	5.42	0.86	0.86
	assign (segid 3A4 and resid 262 and name O)	(segid 3A4 and resid 312 and name O)	6.43	0.67	0.66
55	assign (segid 3A4 and resid 262 and name O)	(segid 3A4 and resid 313 and name CA)	7.34	0.57	0.58
	assign (segid 3A4 and resid 262 and name O)	(segid 3A4 and resid 313 and name CG)	7.14	0.51	0.50
	assign (segid 3A4 and resid 262 and name O)	(segid 3A4 and resid 313 and name N)	6.91	0.70	0.69
	assign (segid 3A4 and resid 262 and name O)	(segid HEM and resid 1 and name CBB)	7.30	0.10	0.11
60	assign (segid 3A4 and resid 263 and name C)	(segid 3A4 and resid 263 and name CB)	2.52	0.02	0.01
	assign (segid 3A4 and resid 263 and name C)	(segid 3A4 and resid 263 and name CG)	3.87	0.06	0.06
	assign (segid 3A4 and resid 263 and name C)	(segid 3A4 and resid 263 and name O)	1.24	0.01	0.01
	assign (segid 3A4 and resid 263 and name C)	(segid 3A4 and resid 264 and name C)	3.05	0.03	0.04
	assign (segid 3A4 and resid 263 and name C)	(segid 3A4 and resid 264 and name CA)	2.44	0.02	0.01
65	assign (segid 3A4 and resid 263 and name C)	(segid 3A4 and resid 264 and name N)	1.32	0.02	0.02
	assign (segid 3A4 and resid 263 and name C)	(segid 3A4 and resid 264 and name O)	3.88	0.06	0.07
	assign (segid 3A4 and resid 263 and name C)	(segid 3A4 and resid 265 and name C)	4.55	0.05	0.06
	assign (segid 3A4 and resid 263 and name C)	(segid 3A4 and resid 265 and name CA)	4.52	0.08	0.09
	assign (segid 3A4 and resid 263 and name C)	(segid 3A4 and resid 265 and name N)	3.35	0.09	0.09
70	assign (segid 3A4 and resid 263 and name C)	(segid 3A4 and resid 265 and name O)	5.63	0.05	0.05
	assign (segid 3A4 and resid 263 and name C)	(segid 3A4 and resid 266 and name C)	4.89	0.08	0.08
	assign (segid 3A4 and resid 263 and name C)	(segid 3A4 and resid 266 and name CA)	4.49	0.08	0.08
	assign (segid 3A4 and resid 263 and name C)	(segid 3A4 and resid 266 and name N)	3.80	0.08	0.08
	assign (segid 3A4 and resid 263 and name C)	(segid 3A4 and resid 266 and name O)	6.11	0.09	0.08
	assign (segid 3A4 and resid 263 and name C)	(segid 3A4 and resid 267 and name C)	6.23	0.16	0.15
75	assign (segid 3A4 and resid 263 and name C)	(segid 3A4 and resid 267 and name CA)	5.17	0.17	0.17
	assign (segid 3A4 and resid 263 and name C)	(segid 3A4 and resid 267 and name CB)	4.81	0.20	0.20
	assign (segid 3A4 and resid 263 and name C)	(segid 3A4 and resid 267 and name N)	4.21	0.12	0.12
	assign (segid 3A4 and resid 263 and name C)	(segid 3A4 and resid 267 and name O)	7.40	0.15	0.15
	assign (segid 3A4 and resid 263 and name C)	(segid 3A4 and resid 268 and name CA)	7.38	0.13	0.12
80	assign (segid 3A4 and resid 263 and name C)	(segid 3A4 and resid 268 and name CB)	7.40	0.12	0.13
	assign (segid 3A4 and resid 263 and name C)	(segid 3A4 and resid 268 and name N)	6.09	0.13	0.14
	assign (segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 263 and name C)	1.53	0.00	0.00
	assign (segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 263 and name CB)	1.53	0.02	0.02

	assign	(segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 263 and name O)	2.53	0.06	0.07
	assign	(segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 264 and name C)	2.39	0.02	0.03
	assign	(segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 264 and name CA)	4.44	0.05	0.04
	assign	(segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 264 and name N)	3.82	0.02	0.01
5	assign	(segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 264 and name O)	2.44	0.02	0.02
	assign	(segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 265 and name C)	5.34	0.08	0.07
	assign	(segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 265 and name N)	5.47	0.09	0.10
	assign	(segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 265 and name O)	5.49	0.12	0.12
	assign	(segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 266 and name C)	4.43	0.10	0.11
10	assign	(segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 266 and name N)	6.60	0.09	0.09
	assign	(segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 266 and name O)	5.70	0.08	0.08
	assign	(segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 267 and name C)	5.04	0.08	0.09
	assign	(segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 267 and name N)	4.51	0.10	0.11
	assign	(segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 267 and name O)	6.88	0.09	0.09
15	assign	(segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 268 and name C)	7.47	0.17	0.17
	assign	(segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 268 and name N)	6.30	0.19	0.19
	assign	(segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 268 and name O)	6.02	0.24	0.24
	assign	(segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 269 and name C)	5.25	0.14	0.13
	assign	(segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 269 and name N)	8.73	0.11	0.11
20	assign	(segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 269 and name O)	8.78	0.11	0.10
	assign	(segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 270 and name C)	7.42	0.13	0.14
	assign	(segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 270 and name N)	9.96	0.09	0.09
	assign	(segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 270 and name O)	10.64	0.14	0.14
	assign	(segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 271 and name C)	9.95	0.17	0.16
25	assign	(segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 271 and name N)	12.27	0.21	0.21
	assign	(segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 271 and name O)	11.82	0.24	0.24
	assign	(segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 272 and name C)	14.23	0.11	0.11
	assign	(segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 272 and name N)	13.92	0.20	0.20
	assign	(segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 272 and name O)	15.33	0.17	0.16
	assign	(segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 273 and name C)	14.91	0.22	0.22
30	assign	(segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 273 and name N)	16.66	0.44	0.43
	assign	(segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 273 and name O)	17.77	0.58	0.59
	assign	(segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 274 and name C)	18.45	0.27	0.26
	assign	(segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 274 and name N)	19.36	0.26	0.25
	assign	(segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 274 and name O)	15.43	0.25	0.25
35	assign	(segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 275 and name C)	14.44	0.26	0.26
	assign	(segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 275 and name N)	14.09	0.28	0.28
	assign	(segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 275 and name O)	13.96	0.35	0.34
	assign	(segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 276 and name C)	17.62	0.31	0.32
40	assign	(segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 276 and name N)	18.86	0.33	0.32
	assign	(segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 276 and name O)	17.96	0.30	0.29
	assign	(segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 277 and name C)	17.89	0.29	0.30
	assign	(segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 277 and name N)	15.00	0.50	0.51
	assign	(segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 277 and name O)	13.53	0.48	0.48
45	assign	(segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 278 and name C)	16.50	0.69	0.68
	assign	(segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 278 and name N)	16.80	0.63	0.63
	assign	(segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 278 and name O)	18.04	0.99	0.99
	assign	(segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 279 and name C)	16.28	0.89	0.88
	assign	(segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 279 and name N)	16.68	0.87	0.87
	assign	(segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 279 and name O)	12.83	0.94	0.95
50	assign	(segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 280 and name C)	12.63	0.96	0.96
	assign	(segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 280 and name N)	13.28	0.88	0.88
	assign	(segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 280 and name O)	14.43	0.88	0.89
	assign	(segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 281 and name C)	15.64	0.90	0.90
	assign	(segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 281 and name N)	11.57	0.91	0.92
55	assign	(segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 281 and name O)	11.23	0.95	0.95
	assign	(segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 282 and name C)	9.18	0.81	0.80
	assign	(segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 282 and name N)	9.22	0.85	0.85
	assign	(segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 282 and name O)	12.02	0.68	0.67
	assign	(segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 283 and name C)	13.42	0.69	0.70
60	assign	(segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 283 and name N)	12.41	0.74	0.75
	assign	(segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 283 and name O)	13.02	0.80	0.80
	assign	(segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 284 and name C)	8.96	0.76	0.77
	assign	(segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 284 and name N)	7.66	0.77	0.77
	assign	(segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 284 and name O)	9.72	0.56	0.56
65	assign	(segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 285 and name C)	10.07	0.51	0.50
	assign	(segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 285 and name N)	13.17	0.59	0.58
	assign	(segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 285 and name O)	14.14	0.59	0.59
	assign	(segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 286 and name C)	12.72	0.66	0.67
	assign	(segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 286 and name N)	12.42	0.67	0.68
70	assign	(segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 286 and name O)	10.49	0.82	0.83
	assign	(segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 287 and name C)	11.87	0.61	0.61
	assign	(segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 287 and name N)	10.66	0.33	0.33
	assign	(segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 287 and name O)	9.42	0.40	0.39
	assign	(segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 288 and name C)	13.86	0.38	0.37
75	assign	(segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 288 and name N)	14.07	0.41	0.41
	assign	(segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 288 and name O)	18.52	0.70	0.71
	assign	(segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 289 and name C)	17.54	0.68	0.67
	assign	(segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 289 and name N)	17.05	0.91	0.91
	assign	(segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 289 and name O)	18.19	0.44	0.44
80	assign	(segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 290 and name C)	18.91	0.76	0.76
	assign	(segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 290 and name N)	18.33	0.70	0.70
	assign	(segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 290 and name O)	15.14	0.72	0.72

	assign (segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 363 and name CB)	14.05	0.66	0.66
	assign (segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 364 and name CA)	16.78	0.77	0.76
	assign (segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 364 and name CB)	18.21	0.76	0.76
	assign (segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 365 and name CA)	15.41	0.91	0.92
	assign (segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 365 and name CB)	14.83	0.97	0.98
5	assign (segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 381 and name CA)	17.74	0.55	0.56
	assign (segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 382 and name CA)	17.74	0.30	0.30
	assign (segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 382 and name CB)	18.95	0.30	0.30
	assign (segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 383 and name CA)	14.18	0.30	0.29
	assign (segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 384 and name CA)	15.16	0.26	0.25
10	assign (segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 384 and name CB)	15.10	0.23	0.23
	assign (segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 385 and name CA)	18.58	0.27	0.27
	assign (segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 391 and name CA)	17.32	0.13	0.14
	assign (segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 391 and name CB)	15.85	0.14	0.15
	assign (segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 392 and name CA)	18.65	0.10	0.10
15	assign (segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 392 and name CB)	19.52	0.17	0.17
	assign (segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 393 and name CA)	15.38	0.10	0.11
	assign (segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 394 and name CA)	14.27	0.23	0.23
	assign (segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 394 and name CB)	15.22	0.34	0.34
	assign (segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 395 and name CA)	15.18	0.28	0.29
20	assign (segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 396 and name CA)	13.50	0.29	0.29
	assign (segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 396 and name CB)	14.02	0.32	0.31
	assign (segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 397 and name CA)	10.16	0.26	0.26
	assign (segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 397 and name CB)	10.20	0.27	0.26
	assign (segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 398 and name CA)	10.60	0.36	0.35
25	assign (segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 398 and name CB)	11.83	0.42	0.42
	assign (segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 399 and name CA)	11.84	0.29	0.30
	assign (segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 399 and name CB)	13.03	0.32	0.32
	assign (segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 400 and name CA)	9.16	0.48	0.49
	assign (segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 400 and name CB)	8.86	0.58	0.58
30	assign (segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 401 and name C)	7.41	0.41	0.41
	assign (segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 401 and name CA)	6.61	0.36	0.36
	assign (segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 401 and name O)	7.06	0.42	0.42
	assign (segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 402 and name CA)	9.65	0.44	0.43
	assign (segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 402 and name CB)	10.96	0.43	0.42
35	assign (segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 403 and name CA)	10.82	0.39	0.40
	assign (segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 403 and name CB)	11.40	0.44	0.45
	assign (segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 404 and name CA)	8.10	0.45	0.45
	assign (segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 404 and name CB)	6.80	0.48	0.47
	assign (segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 405 and name CA)	7.97	0.73	0.74
40	assign (segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 405 and name CB)	7.62	0.79	0.79
	assign (segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 406 and name CA)	11.69	0.74	0.73
	assign (segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 407 and name CA)	12.42	0.52	0.51
	assign (segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 407 and name CB)	12.40	0.51	0.50
	assign (segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 408 and name CA)	10.75	0.48	0.47
45	assign (segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 408 and name CB)	9.36	0.46	0.46
	assign (segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 409 and name CA)	12.50	0.54	0.54
	assign (segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 409 and name CB)	12.27	0.61	0.60
	assign (segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 410 and name CA)	15.57	0.56	0.55
	assign (segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 411 and name CA)	15.94	0.42	0.42
50	assign (segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 411 and name CB)	15.39	0.55	0.55
	assign (segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 412 and name CA)	15.23	0.24	0.23
	assign (segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 413 and name CA)	16.46	0.80	0.80
	assign (segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 414 and name CA)	14.25	0.47	0.48
	assign (segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 415 and name CA)	15.15	0.60	0.61
55	assign (segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 415 and name CB)	16.29	0.87	0.87
	assign (segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 416 and name CA)	15.24	1.07	1.07
	assign (segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 423 and name CA)	17.26	0.86	0.86
	assign (segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 424 and name CA)	15.08	1.48	1.47
	assign (segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 425 and name CA)	14.75	0.48	0.47
60	assign (segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 426 and name CA)	14.18	0.69	0.70
	assign (segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 427 and name CA)	14.40	0.82	0.83
	assign (segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 428 and name CA)	16.60	1.24	1.24
	assign (segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 429 and name CA)	17.14	0.95	0.96
	assign (segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 431 and name CA)	17.15	0.32	0.33
65	assign (segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 433 and name CA)	12.17	0.40	0.39
	assign (segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 434 and name CA)	9.82	0.52	0.51
	assign (segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 435 and name CA)	9.70	0.41	0.41
	assign (segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 436 and name CA)	12.03	0.74	0.74
	assign (segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 437 and name CA)	12.41	0.79	0.80
70	assign (segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 438 and name CA)	11.22	0.72	0.71
	assign (segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 439 and name CA)	13.57	0.21	0.21
	assign (segid 3A4 and resid 263 and name CA)	(segid 3A4 and resid 440 and name CA)	13.44	0.12	0.13
	assign (segid 3A4 and resid 263 and name CB)	(segid 3A4 and resid 263 and name CG)	1.51	0.03	0.04
	assign (segid 3A4 and resid 263 and name CB)	(segid 3A4 and resid 264 and name C)	5.48	0.05	0.04
75	assign (segid 3A4 and resid 263 and name CB)	(segid 3A4 and resid 264 and name CA)	4.51	0.06	0.06
	assign (segid 3A4 and resid 263 and name CB)	(segid 3A4 and resid 264 and name N)	3.17	0.05	0.05
	assign (segid 3A4 and resid 263 and name CB)	(segid 3A4 and resid 264 and name O)	6.33	0.05	0.06
	assign (segid 3A4 and resid 263 and name CB)	(segid 3A4 and resid 265 and name C)	6.90	0.08	0.09
	assign (segid 3A4 and resid 263 and name CB)	(segid 3A4 and resid 265 and name CA)	6.86	0.11	0.11
80	assign (segid 3A4 and resid 263 and name CB)	(segid 3A4 and resid 265 and name N)	5.68	0.11	0.11
	assign (segid 3A4 and resid 263 and name CB)	(segid 3A4 and resid 266 and name C)	6.89	0.09	0.10
	assign (segid 3A4 and resid 263 and name CB)	(segid 3A4 and resid 266 and name CA)	6.41	0.10	0.09

	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 266 and name N)	5.97	0.10	0.10
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 267 and name CA)	7.14	0.22	0.21
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 267 and name CB)	6.58	0.29	0.28
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 267 and name N)	6.29	0.15	0.14
5	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 268 and name CA)	9.79	0.15	0.15
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 268 and name CB)	9.90	0.13	0.12
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 269 and name CA)	11.26	0.11	0.11
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 270 and name CA)	11.66	0.22	0.22
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 270 and name CB)	10.84	0.23	0.24
10	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 271 and name CA)	13.13	0.29	0.28
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 271 and name CB)	12.61	0.30	0.31
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 272 and name CA)	15.34	0.14	0.13
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 272 and name CB)	15.11	0.18	0.17
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 273 and name CA)	16.46	0.22	0.22
15	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 273 and name CB)	16.12	0.28	0.27
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 274 and name CA)	17.55	0.44	0.45
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 274 and name CB)	18.63	0.59	0.60
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 275 and name CA)	19.41	0.32	0.33
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 276 and name CA)	16.43	0.32	0.32
20	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 276 and name CB)	15.53	0.35	0.34
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 277 and name CA)	14.82	0.30	0.31
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 277 and name CB)	14.65	0.34	0.34
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 278 and name CA)	18.25	0.32	0.33
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 279 and name CA)	18.67	0.30	0.30
25	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 279 and name CB)	18.71	0.29	0.28
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 280 and name CA)	15.56	0.47	0.47
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 280 and name CB)	14.11	0.43	0.43
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 281 and name CA)	16.79	0.66	0.66
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 281 and name CB)	17.09	0.61	0.60
30	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 304 and name CA)	16.90	0.87	0.87
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 304 and name CB)	17.34	0.85	0.86
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 305 and name CA)	13.32	0.92	0.93
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 305 and name CB)	12.95	0.95	0.94
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 306 and name CA)	13.80	0.85	0.85
35	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 307 and name CA)	15.29	0.85	0.85
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 307 and name CB)	16.52	0.87	0.87
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 308 and name CA)	12.56	0.88	0.88
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 308 and name CB)	12.14	0.91	0.92
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 309 and name CA)	10.07	0.76	0.76
40	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 309 and name CB)	9.91	0.80	0.79
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 310 and name CA)	13.02	0.66	0.65
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 310 and name CB)	14.39	0.67	0.66
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 311 and name CA)	13.69	0.73	0.73
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 311 and name CB)	14.30	0.78	0.78
45	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 312 and name CA)	10.34	0.76	0.76
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 312 and name CB)	9.01	0.76	0.76
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 313 and name CA)	10.93	0.60	0.59
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 313 and name CB)	11.13	0.54	0.54
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 314 and name CA)	14.48	0.60	0.61
50	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 314 and name CB)	15.46	0.60	0.60
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 315 and name CA)	14.20	0.69	0.68
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 315 and name CB)	13.92	0.69	0.69
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 316 and name CA)	11.91	0.84	0.83
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 317 and name CA)	13.07	0.63	0.63
55	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 318 and name CA)	11.61	0.39	0.40
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 318 and name CB)	10.30	0.45	0.44
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 319 and name CA)	14.62	0.42	0.43
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 319 and name CB)	14.74	0.45	0.45
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 347 and name CA)	18.53	0.69	0.69
60	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 363 and name CA)	16.59	0.73	0.73
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 363 and name CB)	15.49	0.68	0.68
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 364 and name CA)	18.11	0.75	0.76
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 365 and name CA)	16.59	0.89	0.89
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 365 and name CB)	15.94	0.95	0.95
65	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 381 and name CA)	18.83	0.55	0.56
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 382 and name CA)	18.70	0.31	0.31
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 383 and name CA)	15.10	0.30	0.30
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 384 and name CA)	15.76	0.26	0.26
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 384 and name CB)	15.63	0.24	0.25
70	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 385 and name CA)	19.24	0.26	0.27
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 391 and name CA)	17.50	0.15	0.16
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 391 and name CB)	16.08	0.17	0.17
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 392 and name CA)	18.55	0.13	0.13
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 392 and name CB)	19.34	0.18	0.18
75	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 393 and name CA)	15.14	0.11	0.12
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 394 and name CA)	14.33	0.25	0.24
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 394 and name CB)	15.39	0.35	0.34
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 395 and name CA)	15.03	0.28	0.28
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 396 and name CA)	13.01	0.27	0.27
80	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 396 and name CB)	13.44	0.29	0.29
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 397 and name CA)	9.90	0.25	0.25
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 397 and name CB)	10.10	0.27	0.27
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 398 and name CA)	10.61	0.35	0.35

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	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 398 and name CB)	11.95	0.41	0.40
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 399 and name CA)	11.43	0.29	0.28
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 399 and name CB)	12.51	0.32	0.31
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 400 and name CA)	8.41	0.45	0.44
5	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 400 and name CB)	8.03	0.54	0.54
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 400 and name O)	7.01	0.42	0.42
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 401 and name C)	7.21	0.40	0.40
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 401 and name CA)	6.37	0.34	0.34
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 401 and name N)	7.08	0.31	0.31
10	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 401 and name O)	6.88	0.41	0.41
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 402 and name CA)	9.51	0.42	0.43
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 402 and name CB)	10.86	0.41	0.42
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 403 and name CA)	10.18	0.35	0.35
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 403 and name CB)	10.62	0.40	0.40
15	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 404 and name CA)	7.28	0.38	0.39
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 404 and name CB)	5.89	0.38	0.38
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 405 and name CA)	7.80	0.75	0.75
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 405 and name CB)	7.71	0.78	0.78
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 406 and name CA)	11.43	0.69	0.70
20	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 407 and name CA)	11.77	0.47	0.47
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 407 and name CB)	11.59	0.46	0.46
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 408 and name CA)	10.21	0.43	0.44
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 408 and name CB)	8.88	0.41	0.41
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 409 and name CA)	12.38	0.51	0.50
25	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 409 and name CB)	12.30	0.57	0.58
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 410 and name CA)	15.25	0.52	0.52
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 411 and name CA)	15.40	0.39	0.38
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 411 and name CB)	14.73	0.51	0.50
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 412 and name CA)	14.92	0.24	0.24
30	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 413 and name CA)	16.54	0.81	0.82
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 414 and name CA)	14.44	0.50	0.50
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 415 and name CA)	15.53	0.59	0.58
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 415 and name CB)	16.68	0.79	0.78
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 416 and name CA)	15.69	1.05	1.04
35	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 423 and name CA)	18.02	0.79	0.79
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 424 and name CA)	15.92	1.46	1.47
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 425 and name CA)	15.56	0.63	0.62
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 426 and name CA)	15.04	0.77	0.78
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 427 and name CA)	15.16	0.86	0.87
40	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 428 and name CA)	17.30	1.19	1.20
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 429 and name CA)	17.85	0.95	0.95
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 431 and name CA)	17.71	0.37	0.37
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 433 and name CA)	13.01	0.42	0.41
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 434 and name CA)	10.59	0.58	0.57
45	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 435 and name CA)	10.40	0.54	0.55
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 436 and name CA)	12.36	0.99	0.98
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 437 and name CA)	12.59	0.95	0.95
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 438 and name CA)	11.50	0.85	0.84
	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 439 and name CA)	13.63	0.25	0.25
50	assign (segid 3A4 and resid 263 and name CB) (segid 3A4 and resid 440 and name CA)	13.48	0.16	0.17
	assign (segid 3A4 and resid 263 and name CG) (segid 3A4 and resid 264 and name C)	6.85	0.09	0.09
	assign (segid 3A4 and resid 263 and name CG) (segid 3A4 and resid 264 and name CA)	5.96	0.09	0.09
	assign (segid 3A4 and resid 263 and name CG) (segid 3A4 and resid 264 and name N)	4.58	0.10	0.10
	assign (segid 3A4 and resid 263 and name CG) (segid 3A4 and resid 264 and name O)	7.73	0.10	0.10
55	assign (segid 3A4 and resid 263 and name CG) (segid 3A4 and resid 265 and name N)	6.90	0.15	0.15
	assign (segid 3A4 and resid 263 and name CG) (segid 3A4 and resid 266 and name CA)	7.21	0.09	0.09
	assign (segid 3A4 and resid 263 and name CG) (segid 3A4 and resid 266 and name N)	6.91	0.12	0.12
	assign (segid 3A4 and resid 263 and name CG) (segid 3A4 and resid 267 and name N)	7.37	0.18	0.18
	assign (segid 3A4 and resid 263 and name CG) (segid 3A4 and resid 397 and name O)	7.09	0.26	0.25
60	assign (segid 3A4 and resid 263 and name CG) (segid 3A4 and resid 400 and name C)	5.93	0.44	0.43
	assign (segid 3A4 and resid 263 and name CG) (segid 3A4 and resid 400 and name CB)	6.56	0.60	0.59
	assign (segid 3A4 and resid 263 and name CG) (segid 3A4 and resid 400 and name O)	5.69	0.47	0.46
	assign (segid 3A4 and resid 263 and name CG) (segid 3A4 and resid 401 and name C)	6.10	0.48	0.48
	assign (segid 3A4 and resid 263 and name CG) (segid 3A4 and resid 401 and name CA)	5.13	0.41	0.41
65	assign (segid 3A4 and resid 263 and name CG) (segid 3A4 and resid 401 and name N)	5.70	0.36	0.35
	assign (segid 3A4 and resid 263 and name CG) (segid 3A4 and resid 401 and name O)	5.94	0.52	0.51
	assign (segid 3A4 and resid 263 and name CG) (segid 3A4 and resid 404 and name C)	6.93	0.55	0.55
	assign (segid 3A4 and resid 263 and name CG) (segid 3A4 and resid 404 and name CA)	6.52	0.44	0.44
	assign (segid 3A4 and resid 263 and name CG) (segid 3A4 and resid 404 and name CB)	5.09	0.41	0.42
	assign (segid 3A4 and resid 263 and name CG) (segid 3A4 and resid 404 and name N)	7.08	0.43	0.43
70	assign (segid 3A4 and resid 263 and name CG) (segid 3A4 and resid 405 and name N)	6.73	0.71	0.70
	assign (segid 3A4 and resid 263 and name N) (segid 3A4 and resid 263 and name C)	2.46	0.02	0.03
	assign (segid 3A4 and resid 263 and name N) (segid 3A4 and resid 263 and name CA)	1.47	0.02	0.02
	assign (segid 3A4 and resid 263 and name N) (segid 3A4 and resid 263 and name CB)	2.46	0.03	0.03
75	assign (segid 3A4 and resid 263 and name N) (segid 3A4 and resid 263 and name CG)	3.03	0.14	0.14
	assign (segid 3A4 and resid 263 and name N) (segid 3A4 and resid 263 and name O)	3.49	0.04	0.05
	assign (segid 3A4 and resid 263 and name N) (segid 3A4 and resid 264 and name C)	4.71	0.07	0.07
	assign (segid 3A4 and resid 263 and name N) (segid 3A4 and resid 264 and name CA)	4.22	0.05	0.04
	assign (segid 3A4 and resid 263 and name N) (segid 3A4 and resid 264 and name N)	2.81	0.06	0.06
80	assign (segid 3A4 and resid 263 and name N) (segid 3A4 and resid 264 and name O)	5.79	0.06	0.06
	assign (segid 3A4 and resid 263 and name N) (segid 3A4 and resid 265 and name C)	5.56	0.12	0.11
	assign (segid 3A4 and resid 263 and name N) (segid 3A4 and resid 265 and name CA)	5.32	0.16	0.15
	assign (segid 3A4 and resid 263 and name N) (segid 3A4 and resid 265 and name H)	4.33	0.14	0.13

	assign (segid 3A4 and resid 263 and name N)	(segid 3A4 and resid 265 and name O)	6.76	0.12	0.12
	assign (segid 3A4 and resid 263 and name N)	(segid 3A4 and resid 266 and name C)	6.41	0.11	0.10
	assign (segid 3A4 and resid 263 and name N)	(segid 3A4 and resid 266 and name CA)	5.47	0.12	0.13
	assign (segid 3A4 and resid 263 and name N)	(segid 3A4 and resid 266 and name N)	4.72	0.12	0.12
	assign (segid 3A4 and resid 263 and name N)	(segid 3A4 and resid 266 and name O)	7.58	0.11	0.12
5	assign (segid 3A4 and resid 263 and name N)	(segid 3A4 and resid 267 and name CA)	7.32	0.16	0.16
	assign (segid 3A4 and resid 263 and name N)	(segid 3A4 and resid 267 and name CB)	7.17	0.20	0.19
	assign (segid 3A4 and resid 263 and name N)	(segid 3A4 and resid 267 and name N)	6.13	0.13	0.13
	assign (segid 3A4 and resid 263 and name N)	(segid 3A4 and resid 401 and name CA)	6.83	0.45	0.46
	assign (segid 3A4 and resid 263 and name N)	(segid HEM and resid 1 and name CBB)	6.84	0.17	0.16
10	assign (segid 3A4 and resid 263 and name N)	(segid 3A4 and resid 263 and name CB)	3.31	0.04	0.05
	assign (segid 3A4 and resid 263 and name O)	(segid 3A4 and resid 263 and name CG)	4.58	0.06	0.05
	assign (segid 3A4 and resid 263 and name O)	(segid 3A4 and resid 264 and name C)	3.03	0.04	0.03
	assign (segid 3A4 and resid 263 and name O)	(segid 3A4 and resid 264 and name CA)	2.77	0.01	0.01
	assign (segid 3A4 and resid 263 and name O)	(segid 3A4 and resid 264 and name N)	2.25	0.01	0.01
15	assign (segid 3A4 and resid 263 and name O)	(segid 3A4 and resid 264 and name O)	3.48	0.09	0.09
	assign (segid 3A4 and resid 263 and name O)	(segid 3A4 and resid 265 and name C)	4.17	0.05	0.04
	assign (segid 3A4 and resid 263 and name O)	(segid 3A4 and resid 265 and name CA)	4.49	0.08	0.07
	assign (segid 3A4 and resid 263 and name O)	(segid 3A4 and resid 265 and name N)	3.54	0.09	0.09
	assign (segid 3A4 and resid 263 and name O)	(segid 3A4 and resid 265 and name O)	5.08	0.06	0.05
20	assign (segid 3A4 and resid 263 and name O)	(segid 3A4 and resid 266 and name C)	3.87	0.08	0.08
	assign (segid 3A4 and resid 263 and name O)	(segid 3A4 and resid 266 and name CA)	3.77	0.10	0.09
	assign (segid 3A4 and resid 263 and name O)	(segid 3A4 and resid 266 and name N)	3.35	0.10	0.10
	assign (segid 3A4 and resid 263 and name O)	(segid 3A4 and resid 266 and name O)	5.06	0.10	0.09
	assign (segid 3A4 and resid 263 and name O)	(segid 3A4 and resid 267 and name C)	5.14	0.17	0.17
25	assign (segid 3A4 and resid 263 and name O)	(segid 3A4 and resid 267 and name CA)	3.99	0.17	0.17
	assign (segid 3A4 and resid 263 and name O)	(segid 3A4 and resid 267 and name CB)	3.69	0.20	0.21
	assign (segid 3A4 and resid 263 and name O)	(segid 3A4 and resid 267 and name N)	3.08	0.12	0.12
	assign (segid 3A4 and resid 263 and name O)	(segid 3A4 and resid 267 and name O)	6.28	0.16	0.16
	assign (segid 3A4 and resid 263 and name O)	(segid 3A4 and resid 268 and name C)	7.36	0.11	0.11
30	assign (segid 3A4 and resid 263 and name O)	(segid 3A4 and resid 268 and name CA)	6.54	0.13	0.13
	assign (segid 3A4 and resid 263 and name O)	(segid 3A4 and resid 268 and name CB)	6.78	0.13	0.13
	assign (segid 3A4 and resid 263 and name O)	(segid 3A4 and resid 268 and name N)	5.17	0.15	0.14
	assign (segid 3A4 and resid 263 and name O)	(segid 3A4 and resid 269 and name N)	7.04	0.09	0.09
	assign (segid 3A4 and resid 263 and name O)	(segid 3A4 and resid 270 and name CD1)	7.40	0.12	0.11
35	assign (segid 3A4 and resid 263 and name O)	(segid 3A4 and resid 270 and name CG)	7.79	0.08	0.09
	assign (segid 3A4 and resid 263 and name O)	(segid 3A4 and resid 270 and name N)	7.84	0.12	0.13
	assign (segid 3A4 and resid 263 and name O)	(segid 3A4 and resid 264 and name O)	1.24	0.01	0.01
	assign (segid 3A4 and resid 264 and name C)	(segid 3A4 and resid 265 and name C)	3.03	0.05	0.04
40	assign (segid 3A4 and resid 264 and name C)	(segid 3A4 and resid 265 and name CA)	2.45	0.02	0.02
	assign (segid 3A4 and resid 264 and name C)	(segid 3A4 and resid 265 and name N)	1.34	0.01	0.02
	assign (segid 3A4 and resid 264 and name C)	(segid 3A4 and resid 265 and name O)	3.90	0.08	0.07
	assign (segid 3A4 and resid 264 and name C)	(segid 3A4 and resid 266 and name C)	4.58	0.11	0.11
	assign (segid 3A4 and resid 264 and name C)	(segid 3A4 and resid 266 and name CA)	4.46	0.06	0.06
45	assign (segid 3A4 and resid 264 and name C)	(segid 3A4 and resid 266 and name N)	3.29	0.04	0.04
	assign (segid 3A4 and resid 264 and name C)	(segid 3A4 and resid 266 and name O)	5.65	0.12	0.12
	assign (segid 3A4 and resid 264 and name C)	(segid 3A4 and resid 267 and name C)	4.96	0.16	0.16
	assign (segid 3A4 and resid 264 and name C)	(segid 3A4 and resid 267 and name CA)	4.65	0.16	0.15
	assign (segid 3A4 and resid 264 and name C)	(segid 3A4 and resid 267 and name CB)	4.53	0.18	0.17
	assign (segid 3A4 and resid 264 and name C)	(segid 3A4 and resid 267 and name N)	3.88	0.14	0.14
50	assign (segid 3A4 and resid 264 and name C)	(segid 3A4 and resid 267 and name O)	6.17	0.15	0.16
	assign (segid 3A4 and resid 264 and name C)	(segid 3A4 and resid 268 and name C)	6.22	0.15	0.15
	assign (segid 3A4 and resid 264 and name C)	(segid 3A4 and resid 268 and name CA)	5.14	0.14	0.15
	assign (segid 3A4 and resid 264 and name C)	(segid 3A4 and resid 268 and name CB)	4.74	0.15	0.15
	assign (segid 3A4 and resid 264 and name C)	(segid 3A4 and resid 268 and name N)	4.23	0.15	0.14
55	assign (segid 3A4 and resid 264 and name C)	(segid 3A4 and resid 268 and name O)	7.39	0.14	0.14
	assign (segid 3A4 and resid 264 and name C)	(segid 3A4 and resid 269 and name CA)	7.37	0.15	0.15
	assign (segid 3A4 and resid 264 and name C)	(segid 3A4 and resid 269 and name N)	6.10	0.14	0.14
	assign (segid 3A4 and resid 264 and name C)	(segid 3A4 and resid 435 and name C)	7.07	0.28	0.27
	assign (segid 3A4 and resid 264 and name C)	(segid 3A4 and resid 435 and name CA)	6.35	0.19	0.20
60	assign (segid 3A4 and resid 264 and name C)	(segid 3A4 and resid 435 and name N)	6.28	0.27	0.27
	assign (segid 3A4 and resid 264 and name C)	(segid 3A4 and resid 435 and name O)	6.92	0.47	0.47
	assign (segid 3A4 and resid 264 and name CA)	(segid 3A4 and resid 264 and name C)	1.52	0.01	0.01
	assign (segid 3A4 and resid 264 and name CA)	(segid 3A4 and resid 264 and name O)	2.39	0.01	0.01
	assign (segid 3A4 and resid 264 and name CA)	(segid 3A4 and resid 265 and name C)	4.40	0.05	0.05
65	assign (segid 3A4 and resid 264 and name CA)	(segid 3A4 and resid 265 and name CA)	3.82	0.02	0.01
	assign (segid 3A4 and resid 264 and name CA)	(segid 3A4 and resid 265 and name N)	2.45	0.02	0.01
	assign (segid 3A4 and resid 264 and name CA)	(segid 3A4 and resid 265 and name O)	5.34	0.06	0.07
	assign (segid 3A4 and resid 264 and name CA)	(segid 3A4 and resid 266 and name C)	5.51	0.10	0.11
	assign (segid 3A4 and resid 264 and name CA)	(segid 3A4 and resid 266 and name CA)	5.41	0.06	0.06
70	assign (segid 3A4 and resid 264 and name CA)	(segid 3A4 and resid 266 and name N)	4.35	0.05	0.05
	assign (segid 3A4 and resid 264 and name CA)	(segid 3A4 and resid 266 and name O)	6.65	0.10	0.11
	assign (segid 3A4 and resid 264 and name CA)	(segid 3A4 and resid 267 and name C)	5.83	0.19	0.19
	assign (segid 3A4 and resid 264 and name CA)	(segid 3A4 and resid 267 and name CA)	5.26	0.17	0.18
	assign (segid 3A4 and resid 264 and name CA)	(segid 3A4 and resid 267 and name CB)	4.73	0.19	0.19
75	assign (segid 3A4 and resid 264 and name CA)	(segid 3A4 and resid 267 and name N)	4.63	0.14	0.13
	assign (segid 3A4 and resid 264 and name CA)	(segid 3A4 and resid 267 and name O)	7.03	0.20	0.20
	assign (segid 3A4 and resid 264 and name CA)	(segid 3A4 and resid 268 and name C)	7.50	0.18	0.18
	assign (segid 3A4 and resid 264 and name CA)	(segid 3A4 and resid 268 and name CA)	6.32	0.18	0.19
	assign (segid 3A4 and resid 264 and name CA)	(segid 3A4 and resid 268 and name CB)	6.02	0.19	0.19
80	assign (segid 3A4 and resid 264 and name CA)	(segid 3A4 and resid 268 and name N)	5.30	0.18	0.18
	assign (segid 3A4 and resid 264 and name CA)	(segid 3A4 and resid 269 and name CA)	8.74	0.16	0.16
	assign (segid 3A4 and resid 264 and name CA)	(segid 3A4 and resid 269 and name N)	7.46	0.16	0.15

	assign (segid 3A4 and resid 264 and name CA) (segid 3A4 and resid 270 and name CA)	10.07	0.15	0.16
	assign (segid 3A4 and resid 264 and name CA) (segid 3A4 and resid 270 and name CB)	9.74	0.13	0.13
	assign (segid 3A4 and resid 264 and name CA) (segid 3A4 and resid 271 and name CA)	10.62	0.22	0.22
	assign (segid 3A4 and resid 264 and name CA) (segid 3A4 and resid 271 and name CB)	9.81	0.21	0.21
5	assign (segid 3A4 and resid 264 and name CA) (segid 3A4 and resid 272 and name CA)	12.38	0.05	0.05
	assign (segid 3A4 and resid 264 and name CA) (segid 3A4 and resid 272 and name CB)	11.95	0.06	0.07
	assign (segid 3A4 and resid 264 and name CA) (segid 3A4 and resid 273 and name CA)	14.34	0.14	0.15
	assign (segid 3A4 and resid 264 and name CA) (segid 3A4 and resid 273 and name CB)	14.15	0.26	0.26
	assign (segid 3A4 and resid 264 and name CA) (segid 3A4 and resid 274 and name CA)	15.92	0.37	0.36
10	assign (segid 3A4 and resid 264 and name CA) (segid 3A4 and resid 274 and name CB)	16.82	0.53	0.53
	assign (segid 3A4 and resid 264 and name CA) (segid 3A4 and resid 275 and name CA)	18.29	0.20	0.19
	assign (segid 3A4 and resid 264 and name CA) (segid 3A4 and resid 275 and name CB)	19.15	0.19	0.19
	assign (segid 3A4 and resid 264 and name CA) (segid 3A4 and resid 276 and name CA)	15.79	0.21	0.22
	assign (segid 3A4 and resid 264 and name CA) (segid 3A4 and resid 276 and name CB)	14.73	0.22	0.23
15	assign (segid 3A4 and resid 264 and name CA) (segid 3A4 and resid 277 and name CA)	14.45	0.25	0.25
	assign (segid 3A4 and resid 264 and name CA) (segid 3A4 and resid 277 and name CB)	13.98	0.31	0.31
	assign (segid 3A4 and resid 264 and name CA) (segid 3A4 and resid 278 and name CA)	18.12	0.29	0.29
	assign (segid 3A4 and resid 264 and name CA) (segid 3A4 and resid 278 and name CB)	19.16	0.30	0.31
	assign (segid 3A4 and resid 264 and name CA) (segid 3A4 and resid 279 and name CA)	19.04	0.33	0.32
20	assign (segid 3A4 and resid 264 and name CA) (segid 3A4 and resid 279 and name CB)	18.95	0.37	0.37
	assign (segid 3A4 and resid 264 and name CA) (segid 3A4 and resid 280 and name CA)	16.57	0.56	0.55
	assign (segid 3A4 and resid 264 and name CA) (segid 3A4 and resid 280 and name CB)	15.06	0.56	0.56
	assign (segid 3A4 and resid 264 and name CA) (segid 3A4 and resid 281 and name CA)	17.84	0.76	0.76
	assign (segid 3A4 and resid 264 and name CA) (segid 3A4 and resid 281 and name CB)	17.84	0.70	0.70
25	assign (segid 3A4 and resid 264 and name CA) (segid 3A4 and resid 305 and name CA)	15.53	0.95	0.95
	assign (segid 3A4 and resid 264 and name CA) (segid 3A4 and resid 305 and name CB)	15.45	0.95	0.94
	assign (segid 3A4 and resid 264 and name CA) (segid 3A4 and resid 306 and name CA)	16.36	0.87	0.88
	assign (segid 3A4 and resid 264 and name CA) (segid 3A4 and resid 307 and name CA)	16.95	0.93	0.93
	assign (segid 3A4 and resid 264 and name CA) (segid 3A4 and resid 307 and name CB)	18.02	0.95	0.94
30	assign (segid 3A4 and resid 264 and name CA) (segid 3A4 and resid 308 and name CA)	13.67	0.97	0.97
	assign (segid 3A4 and resid 264 and name CA) (segid 3A4 and resid 308 and name CB)	13.27	1.01	1.01
	assign (segid 3A4 and resid 264 and name CA) (segid 3A4 and resid 309 and name CA)	11.93	0.85	0.85
	assign (segid 3A4 and resid 264 and name CA) (segid 3A4 and resid 309 and name CB)	12.31	0.88	0.89
	assign (segid 3A4 and resid 264 and name CA) (segid 3A4 and resid 310 and name CA)	14.50	0.75	0.76
35	assign (segid 3A4 and resid 264 and name CA) (segid 3A4 and resid 310 and name CB)	15.97	0.76	0.76
	assign (segid 3A4 and resid 264 and name CA) (segid 3A4 and resid 311 and name CA)	14.01	0.85	0.85
	assign (segid 3A4 and resid 264 and name CA) (segid 3A4 and resid 311 and name CB)	14.47	0.89	0.90
	assign (segid 3A4 and resid 264 and name CA) (segid 3A4 and resid 312 and name CA)	10.28	0.86	0.85
	assign (segid 3A4 and resid 264 and name CA) (segid 3A4 and resid 312 and name CB)	9.21	0.82	0.83
40	assign (segid 3A4 and resid 264 and name CA) (segid 3A4 and resid 313 and name CA)	11.46	0.64	0.63
	assign (segid 3A4 and resid 264 and name CA) (segid 3A4 and resid 313 and name CB)	12.21	0.58	0.59
	assign (segid 3A4 and resid 264 and name CA) (segid 3A4 and resid 314 and name CA)	14.36	0.67	0.68
	assign (segid 3A4 and resid 264 and name CA) (segid 3A4 and resid 314 and name CB)	15.40	0.71	0.71
	assign (segid 3A4 and resid 264 and name CA) (segid 3A4 and resid 315 and name CA)	12.95	0.77	0.76
45	assign (segid 3A4 and resid 264 and name CA) (segid 3A4 and resid 315 and name CB)	12.53	0.80	0.81
	assign (segid 3A4 and resid 264 and name CA) (segid 3A4 and resid 316 and name CA)	10.35	0.79	0.79
	assign (segid 3A4 and resid 264 and name CA) (segid 3A4 and resid 317 and name CA)	12.36	0.65	0.64
	assign (segid 3A4 and resid 264 and name CA) (segid 3A4 and resid 318 and name CA)	10.87	0.45	0.45
	assign (segid 3A4 and resid 264 and name CA) (segid 3A4 and resid 318 and name CB)	9.86	0.52	0.51
50	assign (segid 3A4 and resid 264 and name CA) (segid 3A4 and resid 319 and name CA)	14.36	0.38	0.37
	assign (segid 3A4 and resid 264 and name CA) (segid 3A4 and resid 319 and name CB)	14.92	0.32	0.31
	assign (segid 3A4 and resid 264 and name CA) (segid 3A4 and resid 347 and name CA)	18.40	0.83	0.84
	assign (segid 3A4 and resid 264 and name CA) (segid 3A4 and resid 347 and name CB)	17.17	1.03	1.03
	assign (segid 3A4 and resid 264 and name CA) (segid 3A4 and resid 351 and name CA)	18.94	0.55	0.54
55	assign (segid 3A4 and resid 264 and name CA) (segid 3A4 and resid 361 and name CA)	18.27	0.90	0.89
	assign (segid 3A4 and resid 264 and name CA) (segid 3A4 and resid 362 and name CA)	17.91	0.85	0.85
	assign (segid 3A4 and resid 264 and name CA) (segid 3A4 and resid 363 and name CA)	15.10	0.88	0.88
	assign (segid 3A4 and resid 264 and name CA) (segid 3A4 and resid 363 and name CB)	13.83	0.82	0.82
	assign (segid 3A4 and resid 264 and name CA) (segid 3A4 and resid 364 and name CA)	17.39	0.88	0.89
60	assign (segid 3A4 and resid 264 and name CA) (segid 3A4 and resid 364 and name CB)	18.79	0.88	0.88
	assign (segid 3A4 and resid 264 and name CA) (segid 3A4 and resid 365 and name CA)	16.79	1.01	1.01
	assign (segid 3A4 and resid 264 and name CA) (segid 3A4 and resid 365 and name CB)	16.26	1.06	1.06
	assign (segid 3A4 and resid 264 and name CA) (segid 3A4 and resid 383 and name CA)	15.92	0.40	0.41
	assign (segid 3A4 and resid 264 and name CA) (segid 3A4 and resid 384 and name CA)	17.42	0.30	0.31
65	assign (segid 3A4 and resid 264 and name CA) (segid 3A4 and resid 384 and name CB)	17.64	0.27	0.27
	assign (segid 3A4 and resid 264 and name CA) (segid 3A4 and resid 391 and name CA)	18.44	0.22	0.23
	assign (segid 3A4 and resid 264 and name CA) (segid 3A4 and resid 393 and name CA)	18.46	0.17	0.18
	assign (segid 3A4 and resid 264 and name CA) (segid 3A4 and resid 394 and name CA)	17.50	0.25	0.26
	assign (segid 3A4 and resid 264 and name CA) (segid 3A4 and resid 394 and name CB)	18.39	0.36	0.36
70	assign (segid 3A4 and resid 264 and name CA) (segid 3A4 and resid 395 and name CA)	18.78	0.28	0.29
	assign (segid 3A4 and resid 264 and name CA) (segid 3A4 and resid 396 and name CA)	17.08	0.30	0.30
	assign (segid 3A4 and resid 264 and name CA) (segid 3A4 and resid 396 and name CB)	17.47	0.33	0.33
	assign (segid 3A4 and resid 264 and name CA) (segid 3A4 and resid 397 and name CA)	13.66	0.28	0.28
	assign (segid 3A4 and resid 264 and name CA) (segid 3A4 and resid 397 and name CB)	13.51	0.29	0.29
75	assign (segid 3A4 and resid 264 and name CA) (segid 3A4 and resid 398 and name CA)	14.29	0.36	0.37
	assign (segid 3A4 and resid 264 and name CA) (segid 3A4 and resid 398 and name CB)	15.47	0.43	0.44
	assign (segid 3A4 and resid 264 and name CA) (segid 3A4 and resid 399 and name CA)	15.65	0.29	0.29
	assign (segid 3A4 and resid 264 and name CA) (segid 3A4 and resid 399 and name CB)	16.81	0.32	0.33
	assign (segid 3A4 and resid 264 and name CA) (segid 3A4 and resid 400 and name CA)	12.85	0.48	0.48
80	assign (segid 3A4 and resid 264 and name CA) (segid 3A4 and resid 400 and name CB)	12.45	0.57	0.58
	assign (segid 3A4 and resid 264 and name CA) (segid 3A4 and resid 401 and name CA)	10.38	0.34	0.35
	assign (segid 3A4 and resid 264 and name CA) (segid 3A4 and resid 402 and name CA)	13.20	0.41	0.40
	assign (segid 3A4 and resid 264 and name CA) (segid 3A4 and resid 402 and name CB)	14.56	0.40	0.40

	assign (segid 3A4 and resid 264 and name O) (segid 3A4 and resid 435 and name N)	6.79	0.24	0.23
	assign (segid 3A4 and resid 264 and name O) (segid 3A4 and resid 435 and name O)	7.30	0.38	0.39
	assign (segid 3A4 and resid 264 and name O) (segid 3A4 and resid 438 and name CA)	7.12	0.33	0.33
	assign (segid 3A4 and resid 265 and name C) (segid 3A4 and resid 265 and name O)	1.24	0.01	0.02
	assign (segid 3A4 and resid 265 and name C) (segid 3A4 and resid 266 and name C)	3.02	0.04	0.04
5	assign (segid 3A4 and resid 265 and name C) (segid 3A4 and resid 266 and name CA)	2.43	0.02	0.03
	assign (segid 3A4 and resid 265 and name C) (segid 3A4 and resid 266 and name N)	1.33	0.01	0.01
	assign (segid 3A4 and resid 265 and name C) (segid 3A4 and resid 266 and name O)	3.83	0.08	0.07
	assign (segid 3A4 and resid 265 and name C) (segid 3A4 and resid 267 and name C)	4.57	0.06	0.05
	assign (segid 3A4 and resid 265 and name C) (segid 3A4 and resid 267 and name CA)	4.50	0.06	0.05
10	assign (segid 3A4 and resid 265 and name C) (segid 3A4 and resid 267 and name CB)	5.31	0.06	0.07
	assign (segid 3A4 and resid 265 and name C) (segid 3A4 and resid 267 and name N)	3.32	0.05	0.05
	assign (segid 3A4 and resid 265 and name C) (segid 3A4 and resid 267 and name O)	5.63	0.06	0.06
	assign (segid 3A4 and resid 265 and name C) (segid 3A4 and resid 268 and name C)	4.92	0.07	0.07
	assign (segid 3A4 and resid 265 and name C) (segid 3A4 and resid 268 and name CA)	4.57	0.06	0.06
15	assign (segid 3A4 and resid 265 and name C) (segid 3A4 and resid 268 and name CB)	4.32	0.10	0.09
	assign (segid 3A4 and resid 265 and name C) (segid 3A4 and resid 268 and name N)	3.85	0.05	0.06
	assign (segid 3A4 and resid 265 and name C) (segid 3A4 and resid 268 and name O)	6.14	0.07	0.07
	assign (segid 3A4 and resid 265 and name C) (segid 3A4 and resid 269 and name C)	6.16	0.08	0.07
	assign (segid 3A4 and resid 265 and name C) (segid 3A4 and resid 269 and name CA)	5.11	0.12	0.11
20	assign (segid 3A4 and resid 265 and name C) (segid 3A4 and resid 269 and name N)	4.20	0.09	0.09
	assign (segid 3A4 and resid 265 and name C) (segid 3A4 and resid 269 and name O)	7.32	0.09	0.08
	assign (segid 3A4 and resid 265 and name C) (segid 3A4 and resid 270 and name CA)	7.34	0.06	0.06
	assign (segid 3A4 and resid 265 and name C) (segid 3A4 and resid 270 and name CB)	7.42	0.06	0.06
	assign (segid 3A4 and resid 265 and name C) (segid 3A4 and resid 270 and name CG)	7.27	0.06	0.05
25	assign (segid 3A4 and resid 265 and name C) (segid 3A4 and resid 270 and name N)	6.04	0.06	0.06
	assign (segid 3A4 and resid 265 and name C) (segid 3A4 and resid 271 and name N)	7.79	0.07	0.07
	assign (segid 3A4 and resid 265 and name C) (segid 3A4 and resid 312 and name C)	7.01	0.66	0.67
	assign (segid 3A4 and resid 265 and name C) (segid 3A4 and resid 312 and name CA)	6.65	0.83	0.82
	assign (segid 3A4 and resid 265 and name C) (segid 3A4 and resid 312 and name CB)	5.84	0.78	0.78
30	assign (segid 3A4 and resid 265 and name C) (segid 3A4 and resid 312 and name O)	6.67	0.56	0.56
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 265 and name C)	1.52	0.00	0.01
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 265 and name O)	2.40	0.02	0.02
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 266 and name C)	4.42	0.05	0.05
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 266 and name CA)	3.81	0.01	0.01
35	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 266 and name N)	2.44	0.02	0.02
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 266 and name O)	5.29	0.08	0.09
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 267 and name C)	5.52	0.06	0.06
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 267 and name CA)	5.50	0.05	0.06
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 267 and name CB)	6.01	0.10	0.11
40	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 267 and name N)	4.43	0.05	0.05
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 267 and name O)	6.63	0.06	0.07
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 268 and name C)	5.75	0.07	0.07
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 268 and name CA)	5.15	0.08	0.07
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 268 and name CB)	4.48	0.12	0.11
45	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 268 and name N)	4.59	0.06	0.05
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 268 and name O)	6.95	0.07	0.08
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 269 and name C)	7.42	0.09	0.09
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 269 and name CA)	6.25	0.11	0.11
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 269 and name N)	5.24	0.10	0.09
50	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 269 and name O)	8.72	0.07	0.08
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 270 and name CB)	8.84	0.08	0.08
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 270 and name N)	7.40	0.08	0.07
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 271 and name CA)	9.88	0.08	0.08
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 271 and name CB)	9.40	0.10	0.10
55	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 272 and name CA)	10.57	0.18	0.18
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 272 and name CB)	9.81	0.25	0.26
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 273 and name CA)	12.30	0.13	0.13
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 273 and name CB)	11.82	0.19	0.19
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 274 and name CA)	14.61	0.39	0.39
60	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 274 and name CB)	15.62	0.50	0.51
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 275 and name CA)	16.58	0.16	0.17
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 275 and name CB)	17.20	0.14	0.15
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 276 and name CA)	14.00	0.19	0.19
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 276 and name CB)	12.71	0.17	0.18
65	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 277 and name CA)	13.55	0.31	0.32
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 277 and name CB)	13.28	0.41	0.41
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 278 and name CA)	17.32	0.31	0.31
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 278 and name CB)	18.23	0.31	0.32
70	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 279 and name CA)	17.84	0.33	0.34
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 279 and name CB)	17.47	0.39	0.40
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 280 and name CA)	15.82	0.56	0.56
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 280 and name CB)	14.34	0.58	0.59
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 281 and name CA)	17.77	0.72	0.71
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 281 and name CB)	17.85	0.66	0.66
75	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 304 and name CA)	17.45	0.88	0.88
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 304 and name CB)	17.54	0.85	0.85
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 305 and name CA)	14.77	0.89	0.89
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 305 and name CB)	15.07	0.85	0.85
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 306 and name CA)	15.33	0.90	0.89
80	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 307 and name CA)	15.10	0.98	0.99
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 307 and name CB)	16.10	1.01	1.00
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 308 and name CA)	11.81	1.01	1.01

	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 308 and name CB)	11.71	1.01	1.00
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 309 and name CA)	10.44	0.91	0.92
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 309 and name CB)	11.25	0.93	0.92
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 310 and name CA)	12.36	0.84	0.85
5	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 310 and name CB)	13.82	0.84	0.85
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 311 and name CA)	11.15	0.95	0.95
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 311 and name CB)	11.61	0.99	0.98
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 312 and name CA)	7.42	0.92	0.93
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 312 and name CB)	6.74	0.88	0.88
10	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 312 and name O)	6.97	0.74	0.73
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 313 and name CA)	8.94	0.64	0.65
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 313 and name CB)	10.03	0.61	0.61
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 314 and name CA)	11.22	0.72	0.72
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 314 and name CB)	12.20	0.78	0.79
15	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 315 and name CA)	9.34	0.80	0.79
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 315 and name CB)	8.88	0.86	0.85
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 316 and name CA)	6.98	0.72	0.71
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 317 and name CA)	9.61	0.51	0.51
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 318 and name CA)	9.05	0.21	0.21
20	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 318 and name CB)	8.40	0.32	0.33
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 319 and name CA)	12.80	0.18	0.18
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 319 and name CB)	13.54	0.17	0.17
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 347 and name CA)	16.57	0.78	0.79
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 347 and name CB)	15.96	0.76	0.76
25	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 348 and name CA)	14.15	0.97	0.96
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 349 and name CA)	17.27	1.11	1.11
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 350 and name CA)	18.46	0.73	0.72
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 351 and name CA)	15.60	0.58	0.58
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 352 and name CA)	16.27	0.70	0.70
30	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 352 and name CB)	15.70	0.80	0.80
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 357 and name CB)	18.19	0.56	0.57
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 360 and name CA)	16.41	0.78	0.78
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 360 and name CB)	17.05	0.77	0.77
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 361 and name CA)	14.48	0.89	0.89
35	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 361 and name CB)	15.16	0.96	0.97
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 362 and name CA)	14.29	0.86	0.85
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 362 and name CB)	15.63	0.89	0.90
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 363 and name CA)	11.69	0.91	0.90
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 363 and name CB)	10.49	0.82	0.82
40	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 364 and name CA)	14.30	0.93	0.93
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 364 and name CB)	15.60	0.92	0.93
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 365 and name CA)	14.21	1.05	1.05
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 365 and name CB)	13.94	1.06	1.07
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 381 and name CA)	16.77	0.74	0.74
45	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 382 and name CA)	17.05	0.50	0.50
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 382 and name CB)	18.03	0.55	0.55
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 383 and name CA)	13.74	0.44	0.44
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 384 and name CA)	15.94	0.35	0.34
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 384 and name CB)	16.31	0.34	0.33
50	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 385 and name CA)	18.77	0.36	0.36
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 391 and name CA)	19.27	0.24	0.24
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 391 and name CB)	17.79	0.24	0.23
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 393 and name CA)	18.76	0.16	0.15
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 394 and name CA)	17.19	0.26	0.25
55	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 394 and name CB)	17.80	0.39	0.38
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 395 and name CA)	18.83	0.30	0.30
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 396 and name CA)	17.85	0.22	0.23
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 396 and name CB)	18.42	0.26	0.25
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 397 and name CA)	14.16	0.22	0.22
60	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 397 and name CB)	13.73	0.24	0.24
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 398 and name CA)	14.27	0.33	0.32
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 398 and name CB)	15.17	0.44	0.44
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 399 and name CA)	16.36	0.22	0.21
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 399 and name CB)	17.66	0.24	0.24
65	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 400 and name CA)	14.26	0.43	0.43
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 400 and name CB)	14.00	0.55	0.54
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 401 and name CA)	11.19	0.31	0.30
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 402 and name CA)	13.67	0.33	0.33
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 402 and name CB)	14.85	0.34	0.34
70	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 403 and name CA)	15.59	0.32	0.32
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 403 and name CB)	16.41	0.37	0.36
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 404 and name CA)	12.97	0.45	0.45
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 404 and name CB)	11.86	0.51	0.51
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 405 and name CA)	11.62	0.60	0.61
75	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 405 and name CB)	10.90	0.68	0.67
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 406 and name CA)	15.25	0.70	0.71
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 407 and name CA)	16.45	0.50	0.51
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 407 and name CB)	16.78	0.47	0.47
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 408 and name CA)	14.12	0.50	0.49
80	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 408 and name CB)	12.63	0.50	0.51
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 409 and name CA)	14.79	0.48	0.48
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 409 and name CB)	14.29	0.55	0.55
	assign (segid 3A4 and resid 265 and name CA) (segid 3A4 and resid 410 and name CA)	18.36	0.49	0.50

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assign (segid 3A4 and resid 265 and name CA ) (segid 3A4 and resid 411 and name CA ) 18.85 0.35 0.35
assign (segid 3A4 and resid 265 and name CA ) (segid 3A4 and resid 411 and name CB ) 18.60 0.50 0.50
assign (segid 3A4 and resid 265 and name CA ) (segid 3A4 and resid 412 and name CA ) 17.15 0.20 0.21
assign (segid 3A4 and resid 265 and name CA ) (segid 3A4 and resid 413 and name CA ) 16.79 0.93 0.92
assign (segid 3A4 and resid 265 and name CA ) (segid 3A4 and resid 414 and name CA ) 13.99 0.51 0.51
5 assign (segid 3A4 and resid 265 and name CA ) (segid 3A4 and resid 415 and name CA ) 13.74 0.87 0.86
assign (segid 3A4 and resid 265 and name CA ) (segid 3A4 and resid 415 and name CB ) 14.74 1.41 1.40
assign (segid 3A4 and resid 265 and name CA ) (segid 3A4 and resid 416 and name CA ) 13.08 1.06 1.06
assign (segid 3A4 and resid 265 and name CA ) (segid 3A4 and resid 417 and name CA ) 16.00 0.96 0.96
10 assign (segid 3A4 and resid 265 and name CA ) (segid 3A4 and resid 423 and name CA ) 13.18 1.00 1.00
assign (segid 3A4 and resid 265 and name CA ) (segid 3A4 and resid 424 and name CA ) 10.79 1.48 1.47
assign (segid 3A4 and resid 265 and name CA ) (segid 3A4 and resid 425 and name CA ) 10.57 0.52 0.52
assign (segid 3A4 and resid 265 and name CA ) (segid 3A4 and resid 426 and name CA ) 10.02 0.57 0.56
assign (segid 3A4 and resid 265 and name CA ) (segid 3A4 and resid 427 and name CA ) 10.84 1.03 1.03
15 assign (segid 3A4 and resid 265 and name CA ) (segid 3A4 and resid 428 and name CA ) 13.34 1.21 1.22
assign (segid 3A4 and resid 265 and name CA ) (segid 3A4 and resid 429 and name CA ) 14.23 0.90 0.90
assign (segid 3A4 and resid 265 and name CA ) (segid 3A4 and resid 430 and name CA ) 16.01 0.77 0.77
assign (segid 3A4 and resid 265 and name CA ) (segid 3A4 and resid 431 and name CA ) 15.58 0.45 0.45
assign (segid 3A4 and resid 265 and name CA ) (segid 3A4 and resid 433 and name CA ) 9.54 0.60 0.60
20 assign (segid 3A4 and resid 265 and name CA ) (segid 3A4 and resid 434 and name C ) 6.96 0.27 0.28
assign (segid 3A4 and resid 265 and name CA ) (segid 3A4 and resid 434 and name CA ) 7.14 0.41 0.41
assign (segid 3A4 and resid 265 and name CA ) (segid 3A4 and resid 435 and name CA ) 6.54 0.23 0.23
assign (segid 3A4 and resid 265 and name CA ) (segid 3A4 and resid 435 and name N ) 6.25 0.19 0.20
assign (segid 3A4 and resid 265 and name CA ) (segid 3A4 and resid 436 and name CA ) 9.85 0.48 0.47
25 assign (segid 3A4 and resid 265 and name CA ) (segid 3A4 and resid 437 and name CA ) 10.58 0.50 0.50
assign (segid 3A4 and resid 265 and name CA ) (segid 3A4 and resid 438 and name CA ) 9.29 0.25 0.25
assign (segid 3A4 and resid 265 and name CA ) (segid 3A4 and resid 439 and name CA ) 12.30 0.23 0.23
assign (segid 3A4 and resid 265 and name CA ) (segid 3A4 and resid 440 and name CA ) 12.73 0.19 0.19
30 assign (segid 3A4 and resid 265 and name N ) (segid 3A4 and resid 265 and name C ) 2.44 0.02 0.02
assign (segid 3A4 and resid 265 and name N ) (segid 3A4 and resid 265 and name CA ) 1.46 0.01 0.00
assign (segid 3A4 and resid 265 and name N ) (segid 3A4 and resid 265 and name O ) 3.50 0.05 0.05
assign (segid 3A4 and resid 265 and name N ) (segid 3A4 and resid 266 and name C ) 4.71 0.07 0.07
35 assign (segid 3A4 and resid 265 and name N ) (segid 3A4 and resid 266 and name CA ) 4.18 0.05 0.05
assign (segid 3A4 and resid 265 and name N ) (segid 3A4 and resid 266 and name N ) 2.79 0.06 0.05
assign (segid 3A4 and resid 265 and name N ) (segid 3A4 and resid 266 and name O ) 5.77 0.08 0.09
40 assign (segid 3A4 and resid 265 and name N ) (segid 3A4 and resid 267 and name C ) 5.68 0.09 0.09
assign (segid 3A4 and resid 265 and name N ) (segid 3A4 and resid 267 and name CA ) 5.40 0.09 0.10
assign (segid 3A4 and resid 265 and name N ) (segid 3A4 and resid 267 and name CB ) 5.56 0.14 0.14
assign (segid 3A4 and resid 265 and name N ) (segid 3A4 and resid 267 and name N ) 4.37 0.09 0.09
45 assign (segid 3A4 and resid 265 and name N ) (segid 3A4 and resid 267 and name O ) 6.89 0.10 0.09
assign (segid 3A4 and resid 265 and name N ) (segid 3A4 and resid 268 and name C ) 6.53 0.10 0.10
assign (segid 3A4 and resid 265 and name N ) (segid 3A4 and resid 268 and name CA ) 5.67 0.10 0.10
assign (segid 3A4 and resid 265 and name N ) (segid 3A4 and resid 268 and name CB ) 5.10 0.12 0.12
50 assign (segid 3A4 and resid 265 and name N ) (segid 3A4 and resid 268 and name N ) 4.87 0.09 0.09
assign (segid 3A4 and resid 265 and name N ) (segid 3A4 and resid 268 and name O ) 7.74 0.10 0.10
assign (segid 3A4 and resid 265 and name N ) (segid 3A4 and resid 269 and name CA ) 7.31 0.12 0.12
assign (segid 3A4 and resid 265 and name N ) (segid 3A4 and resid 269 and name N ) 6.18 0.12 0.11
55 assign (segid 3A4 and resid 265 and name N ) (segid 3A4 and resid 434 and name C ) 6.80 0.35 0.35
assign (segid 3A4 and resid 265 and name N ) (segid 3A4 and resid 435 and name C ) 7.16 0.24 0.25
assign (segid 3A4 and resid 265 and name N ) (segid 3A4 and resid 435 and name CA ) 6.27 0.14 0.14
60 assign (segid 3A4 and resid 265 and name N ) (segid 3A4 and resid 435 and name N ) 5.96 0.22 0.21
assign (segid 3A4 and resid 265 and name N ) (segid 3A4 and resid 435 and name O ) 7.09 0.44 0.43
assign (segid 3A4 and resid 265 and name O ) (segid 3A4 and resid 266 and name C ) 2.95 0.08 0.08
assign (segid 3A4 and resid 265 and name O ) (segid 3A4 and resid 266 and name CA ) 2.76 0.04 0.03
65 assign (segid 3A4 and resid 265 and name O ) (segid 3A4 and resid 266 and name N ) 2.25 0.02 0.01
assign (segid 3A4 and resid 265 and name O ) (segid 3A4 and resid 267 and name C ) 3.38 0.12 0.12
assign (segid 3A4 and resid 265 and name O ) (segid 3A4 and resid 267 and name CA ) 4.40 0.12 0.11
70 assign (segid 3A4 and resid 265 and name O ) (segid 3A4 and resid 267 and name CB ) 5.45 0.15 0.15
assign (segid 3A4 and resid 265 and name O ) (segid 3A4 and resid 267 and name N ) 3.45 0.09 0.09
assign (segid 3A4 and resid 265 and name O ) (segid 3A4 and resid 267 and name O ) 5.02 0.14 0.14
75 assign (segid 3A4 and resid 265 and name O ) (segid 3A4 and resid 268 and name C ) 3.88 0.11 0.11
assign (segid 3A4 and resid 265 and name O ) (segid 3A4 and resid 268 and name CA ) 3.80 0.12 0.13
assign (segid 3A4 and resid 265 and name O ) (segid 3A4 and resid 268 and name CB ) 3.64 0.15 0.15
80 assign (segid 3A4 and resid 265 and name O ) (segid 3A4 and resid 268 and name N ) 3.35 0.13 0.13
assign (segid 3A4 and resid 265 and name O ) (segid 3A4 and resid 268 and name O ) 5.06 0.10 0.11
assign (segid 3A4 and resid 265 and name O ) (segid 3A4 and resid 269 and name C ) 5.06 0.09 0.09
assign (segid 3A4 and resid 265 and name O ) (segid 3A4 and resid 269 and name CA ) 3.92 0.11 0.11
assign (segid 3A4 and resid 265 and name O ) (segid 3A4 and resid 269 and name N ) 3.05 0.11 0.11
70 assign (segid 3A4 and resid 265 and name O ) (segid 3A4 and resid 269 and name O ) 6.18 0.09 0.10
assign (segid 3A4 and resid 265 and name O ) (segid 3A4 and resid 270 and name C ) 7.28 0.12 0.12
assign (segid 3A4 and resid 265 and name O ) (segid 3A4 and resid 270 and name CA ) 6.48 0.09 0.09
assign (segid 3A4 and resid 265 and name O ) (segid 3A4 and resid 270 and name CB ) 6.76 0.10 0.10
75 assign (segid 3A4 and resid 265 and name O ) (segid 3A4 and resid 270 and name CD1) 7.34 0.19 0.19
assign (segid 3A4 and resid 265 and name O ) (segid 3A4 and resid 270 and name CD2) 7.77 0.08 0.08
assign (segid 3A4 and resid 265 and name O ) (segid 3A4 and resid 270 and name CG ) 6.73 0.08 0.07
80 assign (segid 3A4 and resid 265 and name O ) (segid 3A4 and resid 270 and name N ) 5.10 0.08 0.08
assign (segid 3A4 and resid 265 and name O ) (segid 3A4 and resid 271 and name N ) 6.89 0.11 0.10
assign (segid 3A4 and resid 265 and name O ) (segid 3A4 and resid 312 and name CA ) 6.71 0.68 0.68
assign (segid 3A4 and resid 265 and name O ) (segid 3A4 and resid 312 and name CB ) 6.05 0.64 0.64
assign (segid 3A4 and resid 265 and name O ) (segid 3A4 and resid 312 and name O ) 6.88 0.40 0.41
assign (segid 3A4 and resid 266 and name C ) (segid 3A4 and resid 266 and name O ) 1.23 0.00 0.01
assign (segid 3A4 and resid 266 and name C ) (segid 3A4 and resid 267 and name C ) 3.06 0.05 0.04

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	assign (segid 3A4 and resid 266 and name C)	(segid 3A4 and resid 267 and name CA)	2.44	0.02	0.01
	assign (segid 3A4 and resid 266 and name C)	(segid 3A4 and resid 267 and name CB)	3.71	0.02	0.02
	assign (segid 3A4 and resid 266 and name C)	(segid 3A4 and resid 267 and name N)	1.32	0.01	0.02
	assign (segid 3A4 and resid 266 and name C)	(segid 3A4 and resid 267 and name O)	3.90	0.08	0.07
	assign (segid 3A4 and resid 266 and name C)	(segid 3A4 and resid 268 and name C)	4.57	0.05	0.05
5	assign (segid 3A4 and resid 266 and name C)	(segid 3A4 and resid 268 and name CA)	4.51	0.05	0.05
	assign (segid 3A4 and resid 266 and name C)	(segid 3A4 and resid 268 and name CB)	5.22	0.08	0.08
	assign (segid 3A4 and resid 266 and name C)	(segid 3A4 and resid 268 and name N)	3.34	0.04	0.05
	assign (segid 3A4 and resid 266 and name C)	(segid 3A4 and resid 268 and name O)	5.62	0.07	0.08
	assign (segid 3A4 and resid 266 and name C)	(segid 3A4 and resid 269 and name C)	4.87	0.07	0.06
10	assign (segid 3A4 and resid 266 and name C)	(segid 3A4 and resid 269 and name CA)	4.57	0.09	0.08
	assign (segid 3A4 and resid 266 and name C)	(segid 3A4 and resid 269 and name N)	3.86	0.07	0.07
	assign (segid 3A4 and resid 266 and name C)	(segid 3A4 and resid 269 and name O)	6.08	0.06	0.06
	assign (segid 3A4 and resid 266 and name C)	(segid 3A4 and resid 270 and name C)	6.10	0.07	0.08
	assign (segid 3A4 and resid 266 and name C)	(segid 3A4 and resid 270 and name CA)	5.10	0.06	0.06
15	assign (segid 3A4 and resid 266 and name C)	(segid 3A4 and resid 270 and name CB)	4.75	0.06	0.07
	assign (segid 3A4 and resid 266 and name C)	(segid 3A4 and resid 270 and name CD1)	4.71	0.21	0.21
	assign (segid 3A4 and resid 266 and name C)	(segid 3A4 and resid 270 and name CD2)	5.79	0.09	0.09
	assign (segid 3A4 and resid 266 and name C)	(segid 3A4 and resid 270 and name CG)	4.51	0.07	0.06
	assign (segid 3A4 and resid 266 and name C)	(segid 3A4 and resid 270 and name N)	4.15	0.06	0.07
20	assign (segid 3A4 and resid 266 and name C)	(segid 3A4 and resid 270 and name O)	7.27	0.08	0.08
	assign (segid 3A4 and resid 266 and name C)	(segid 3A4 and resid 271 and name CA)	7.19	0.08	0.08
	assign (segid 3A4 and resid 266 and name C)	(segid 3A4 and resid 271 and name CB)	7.15	0.09	0.10
	assign (segid 3A4 and resid 266 and name C)	(segid 3A4 and resid 271 and name N)	5.93	0.07	0.08
	assign (segid 3A4 and resid 266 and name C)	(segid 3A4 and resid 271 and name O)	7.73	0.09	0.08
25	assign (segid 3A4 and resid 266 and name C)	(segid 3A4 and resid 272 and name N)	7.13	0.48	0.49
	assign (segid 3A4 and resid 266 and name C)	(segid 3A4 and resid 312 and name CA)	6.02	0.40	0.40
	assign (segid 3A4 and resid 266 and name C)	(segid 3A4 and resid 312 and name CB)	1.53	0.01	0.02
	assign (segid 3A4 and resid 266 and name C)	(segid 3A4 and resid 266 and name C)	2.40	0.03	0.02
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 266 and name O)	4.45	0.04	0.04
30	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 267 and name C)	3.82	0.02	0.02
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 267 and name CA)	4.87	0.02	0.02
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 267 and name CB)	2.44	0.03	0.04
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 267 and name N)	5.37	0.08	0.07
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 267 and name O)	5.55	0.02	0.02
35	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 268 and name C)	5.51	0.05	0.04
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 268 and name CA)	5.88	0.09	0.09
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 268 and name CB)	4.44	0.04	0.04
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 268 and name N)	6.67	0.05	0.05
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 268 and name O)	5.76	0.04	0.04
40	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 269 and name C)	5.21	0.08	0.07
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 269 and name CA)	4.64	0.05	0.05
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 269 and name N)	6.94	0.03	0.03
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 269 and name O)	7.40	0.07	0.08
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 270 and name C)	6.27	0.04	0.05
45	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 270 and name CA)	5.98	0.03	0.03
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 270 and name CB)	5.62	0.20	0.20
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 270 and name CD1)	6.56	0.12	0.11
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 270 and name CD2)	5.46	0.04	0.04
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 270 and name CG)	5.24	0.05	0.04
50	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 270 and name N)	8.60	0.08	0.08
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 271 and name CA)	8.58	0.09	0.10
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 271 and name CB)	7.31	0.07	0.08
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 271 and name N)	9.88	0.13	0.12
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 272 and name CA)	9.53	0.25	0.25
55	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 272 and name CB)	10.57	0.11	0.10
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 273 and name CA)	10.00	0.18	0.18
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 273 and name CB)	12.36	0.44	0.44
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 274 and name CA)	13.56	0.55	0.56
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 274 and name CB)	13.95	0.23	0.22
60	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 275 and name CA)	14.70	0.21	0.21
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 275 and name CB)	10.98	0.22	0.23
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 276 and name CA)	9.82	0.22	0.23
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 276 and name CB)	10.35	0.29	0.28
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 277 and name CA)	10.29	0.36	0.37
65	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 277 and name CB)	14.07	0.29	0.28
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 278 and name CA)	15.12	0.31	0.30
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 278 and name CB)	14.35	0.32	0.32
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 279 and name CA)	14.05	0.37	0.37
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 279 and name CB)	12.10	0.55	0.55
70	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 280 and name CA)	10.62	0.57	0.56
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 281 and name CA)	14.16	0.67	0.66
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 281 and name CB)	14.37	0.61	0.60
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 282 and name CA)	17.29	0.63	0.62
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 303 and name CA)	16.41	0.91	0.91
75	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 303 and name CB)	17.75	0.93	0.92
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 304 and name CA)	13.83	0.88	0.88
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 304 and name CB)	13.90	0.87	0.86
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 305 and name CA)	11.12	0.89	0.88
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 305 and name CB)	11.41	0.82	0.83
80	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 306 and name CA)	12.12	0.84	0.83
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 307 and name CA)	12.04	0.93	0.92
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 307 and name CB)	12.96	0.96	0.96

	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 308 and name CA)	8.53	0.98	0.99
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 308 and name CB)	8.17	1.01	1.02
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 309 and name CA)	7.64	0.78	0.78
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 309 and name CB)	8.47	0.81	0.80
5	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 310 and name CA)	10.26	0.63	0.64
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 310 and name CB)	11.63	0.67	0.67
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 311 and name CA)	9.25	0.73	0.73
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 311 and name CB)	9.43	0.82	0.82
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 312 and name C)	6.64	0.41	0.42
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 312 and name CA)	5.92	0.58	0.57
10	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 312 and name CB)	4.78	0.51	0.51
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 312 and name N)	6.94	0.70	0.69
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 312 and name O)	6.73	0.38	0.37
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 313 and name CA)	8.46	0.29	0.30
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 313 and name CB)	9.33	0.28	0.27
15	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 314 and name CA)	10.92	0.43	0.44
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 314 and name CB)	11.57	0.50	0.50
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 315 and name CA)	9.58	0.56	0.56
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 315 and name CB)	8.80	0.61	0.61
20	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 316 and name CA)	8.45	0.70	0.70
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 317 and name CA)	11.08	0.54	0.54
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 318 and name CA)	11.29	0.24	0.24
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 318 and name CB)	10.53	0.32	0.31
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 319 and name CA)	14.92	0.25	0.26
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 319 and name CB)	15.41	0.32	0.32
25	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 347 and name CA)	17.95	0.59	0.60
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 347 and name CB)	17.30	0.55	0.55
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 348 and name CA)	15.77	0.84	0.83
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 351 and name CA)	16.01	0.36	0.37
30	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 352 and name CA)	16.91	0.60	0.60
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 352 and name CB)	16.64	0.71	0.71
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 357 and name CA)	19.01	0.40	0.41
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 357 and name CB)	17.64	0.40	0.40
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 359 and name CA)	18.60	0.66	0.66
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 359 and name CB)	18.52	0.71	0.71
35	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 360 and name CA)	16.32	0.61	0.62
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 360 and name CB)	17.19	0.63	0.63
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 361 and name CA)	14.81	0.77	0.76
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 361 and name CB)	15.74	0.87	0.87
40	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 362 and name CA)	13.72	0.71	0.72
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 362 and name CB)	14.86	0.78	0.78
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 363 and name CA)	10.44	0.75	0.75
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 363 and name CB)	9.24	0.69	0.69
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 364 and name CA)	12.22	0.82	0.83
45	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 364 and name CB)	13.67	0.81	0.81
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 365 and name CA)	11.41	1.00	0.99
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 365 and name CB)	10.87	1.06	1.05
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 381 and name CA)	16.31	0.52	0.52
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 382 and name CA)	17.22	0.27	0.27
50	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 382 and name CB)	18.41	0.32	0.32
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 383 and name CA)	14.14	0.26	0.26
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 384 and name CA)	16.16	0.24	0.25
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 384 and name CB)	16.21	0.26	0.25
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 385 and name CA)	19.34	0.26	0.26
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 391 and name CA)	19.52	0.19	0.18
55	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 391 and name CB)	17.99	0.19	0.19
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 393 and name CA)	18.50	0.18	0.18
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 394 and name CA)	16.50	0.25	0.25
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 394 and name CB)	17.08	0.36	0.36
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 395 and name CA)	17.48	0.34	0.34
60	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 396 and name CA)	16.71	0.30	0.31
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 396 and name CB)	17.53	0.33	0.33
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 397 and name CA)	13.25	0.32	0.31
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 397 and name CB)	13.09	0.30	0.31
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 398 and name CA)	12.46	0.36	0.35
65	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 398 and name CB)	13.29	0.44	0.44
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 399 and name CA)	14.24	0.27	0.28
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 399 and name CB)	15.66	0.28	0.28
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 400 and name CA)	12.53	0.49	0.50
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 400 and name CB)	12.66	0.60	0.60
70	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 401 and name CA)	9.03	0.40	0.39
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 402 and name CA)	10.72	0.33	0.34
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 402 and name CB)	11.91	0.34	0.33
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 403 and name CA)	12.85	0.36	0.36
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 403 and name CB)	13.90	0.41	0.40
75	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 404 and name CA)	10.53	0.53	0.53
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 404 and name CB)	9.73	0.65	0.64
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 405 and name CA)	8.45	0.53	0.54
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 405 and name CB)	7.54	0.62	0.62
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 406 and name CA)	11.87	0.68	0.67
80	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 407 and name CA)	13.52	0.48	0.48
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 407 and name CB)	14.05	0.45	0.45
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 408 and name CA)	11.47	0.38	0.37

	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 408 and name CB)	10.10	0.40	0.40
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 409 and name CA)	11.66	0.41	0.42
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 409 and name CB)	10.98	0.49	0.48
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 410 and name CA)	15.17	0.44	0.45
5	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 411 and name CA)	16.18	0.34	0.33
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 411 and name CB)	16.08	0.48	0.49
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 412 and name CA)	14.75	0.33	0.34
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 413 and name CA)	14.72	0.94	0.93
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 414 and name CA)	12.49	0.62	0.62
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 415 and name CA)	13.04	0.67	0.68
10	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 415 and name CB)	14.11	1.02	1.01
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 416 and name CA)	13.29	1.15	1.15
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 417 and name CA)	16.61	0.97	0.96
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 423 and name CA)	15.33	1.12	1.11
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 424 and name CA)	13.29	1.56	1.56
15	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 425 and name CA)	13.62	0.74	0.73
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 426 and name CA)	13.55	0.59	0.59
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 427 and name CA)	14.57	0.99	0.98
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 428 and name CA)	17.07	1.22	1.22
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 429 and name CA)	17.83	0.93	0.93
20	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 431 and name CA)	18.62	0.43	0.44
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 433 and name CA)	12.87	0.67	0.66
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 434 and name CA)	10.76	0.42	0.42
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 435 and name CA)	10.15	0.23	0.23
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 436 and name CA)	13.16	0.53	0.52
25	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 437 and name CA)	13.35	0.53	0.53
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 438 and name CA)	11.30	0.32	0.33
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 439 and name CA)	13.59	0.21	0.22
	assign (segid 3A4 and resid 266 and name CA)	(segid 3A4 and resid 440 and name CA)	12.94	0.21	0.22
	assign (segid 3A4 and resid 266 and name N)	(segid 3A4 and resid 266 and name C)	2.47	0.02	0.01
30	assign (segid 3A4 and resid 266 and name N)	(segid 3A4 and resid 266 and name CA)	1.45	0.01	0.01
	assign (segid 3A4 and resid 266 and name N)	(segid 3A4 and resid 266 and name O)	3.48	0.04	0.05
	assign (segid 3A4 and resid 266 and name N)	(segid 3A4 and resid 267 and name C)	4.74	0.05	0.05
	assign (segid 3A4 and resid 266 and name N)	(segid 3A4 and resid 267 and name CA)	4.25	0.04	0.04
	assign (segid 3A4 and resid 266 and name N)	(segid 3A4 and resid 267 and name CB)	5.03	0.04	0.05
35	assign (segid 3A4 and resid 266 and name N)	(segid 3A4 and resid 267 and name N)	2.85	0.05	0.05
	assign (segid 3A4 and resid 266 and name N)	(segid 3A4 and resid 267 and name O)	5.82	0.05	0.06
	assign (segid 3A4 and resid 266 and name N)	(segid 3A4 and resid 268 and name C)	5.67	0.04	0.05
	assign (segid 3A4 and resid 266 and name N)	(segid 3A4 and resid 268 and name CA)	5.36	0.05	0.06
	assign (segid 3A4 and resid 266 and name N)	(segid 3A4 and resid 268 and name CB)	5.38	0.08	0.08
40	assign (segid 3A4 and resid 266 and name N)	(segid 3A4 and resid 268 and name N)	4.36	0.05	0.06
	assign (segid 3A4 and resid 266 and name N)	(segid 3A4 and resid 268 and name O)	6.88	0.04	0.04
	assign (segid 3A4 and resid 266 and name N)	(segid 3A4 and resid 269 and name C)	6.50	0.06	0.06
	assign (segid 3A4 and resid 266 and name N)	(segid 3A4 and resid 269 and name CA)	5.68	0.11	0.10
	assign (segid 3A4 and resid 266 and name N)	(segid 3A4 and resid 269 and name N)	4.88	0.07	0.08
45	assign (segid 3A4 and resid 266 and name N)	(segid 3A4 and resid 269 and name O)	7.70	0.06	0.05
	assign (segid 3A4 and resid 266 and name N)	(segid 3A4 and resid 270 and name CA)	7.32	0.04	0.05
	assign (segid 3A4 and resid 266 and name N)	(segid 3A4 and resid 270 and name CB)	7.15	0.04	0.05
	assign (segid 3A4 and resid 266 and name N)	(segid 3A4 and resid 270 and name CD1)	6.98	0.20	0.20
	assign (segid 3A4 and resid 266 and name N)	(segid 3A4 and resid 270 and name CG)	6.79	0.04	0.04
50	assign (segid 3A4 and resid 266 and name N)	(segid 3A4 and resid 270 and name N)	6.16	0.06	0.05
	assign (segid 3A4 and resid 266 and name N)	(segid 3A4 and resid 312 and name C)	6.69	0.62	0.63
	assign (segid 3A4 and resid 266 and name N)	(segid 3A4 and resid 312 and name CA)	6.26	0.80	0.80
	assign (segid 3A4 and resid 266 and name N)	(segid 3A4 and resid 312 and name CB)	5.23	0.76	0.75
	assign (segid 3A4 and resid 266 and name N)	(segid 3A4 and resid 312 and name O)	6.56	0.54	0.54
55	assign (segid 3A4 and resid 266 and name N)	(segid 3A4 and resid 267 and name C)	3.03	0.10	0.10
	assign (segid 3A4 and resid 266 and name O)	(segid 3A4 and resid 267 and name CA)	2.77	0.05	0.05
	assign (segid 3A4 and resid 266 and name O)	(segid 3A4 and resid 267 and name CB)	4.25	0.04	0.05
	assign (segid 3A4 and resid 266 and name O)	(segid 3A4 and resid 267 and name N)	2.25	0.03	0.02
	assign (segid 3A4 and resid 266 and name O)	(segid 3A4 and resid 267 and name O)	3.51	0.13	0.13
60	assign (segid 3A4 and resid 266 and name O)	(segid 3A4 and resid 268 and name C)	4.13	0.15	0.15
	assign (segid 3A4 and resid 266 and name O)	(segid 3A4 and resid 268 and name CA)	4.44	0.13	0.13
	assign (segid 3A4 and resid 266 and name O)	(segid 3A4 and resid 268 and name CB)	5.36	0.16	0.16
	assign (segid 3A4 and resid 266 and name O)	(segid 3A4 and resid 268 and name N)	3.51	0.10	0.11
	assign (segid 3A4 and resid 266 and name O)	(segid 3A4 and resid 268 and name O)	5.02	0.17	0.18
65	assign (segid 3A4 and resid 266 and name O)	(segid 3A4 and resid 269 and name C)	3.81	0.12	0.11
	assign (segid 3A4 and resid 266 and name O)	(segid 3A4 and resid 269 and name CA)	3.76	0.15	0.15
	assign (segid 3A4 and resid 266 and name O)	(segid 3A4 and resid 269 and name N)	3.33	0.17	0.16
	assign (segid 3A4 and resid 266 and name O)	(segid 3A4 and resid 269 and name O)	4.99	0.11	0.10
	assign (segid 3A4 and resid 266 and name O)	(segid 3A4 and resid 270 and name C)	5.04	0.08	0.08
70	assign (segid 3A4 and resid 266 and name O)	(segid 3A4 and resid 270 and name CA)	3.95	0.06	0.05
	assign (segid 3A4 and resid 266 and name O)	(segid 3A4 and resid 270 and name CB)	3.70	0.07	0.07
	assign (segid 3A4 and resid 266 and name O)	(segid 3A4 and resid 270 and name CD1)	3.98	0.25	0.25
	assign (segid 3A4 and resid 266 and name O)	(segid 3A4 and resid 270 and name CD2)	4.73	0.08	0.07
	assign (segid 3A4 and resid 266 and name O)	(segid 3A4 and resid 270 and name CG)	3.49	0.09	0.09
75	assign (segid 3A4 and resid 266 and name O)	(segid 3A4 and resid 270 and name N)	3.01	0.08	0.08
	assign (segid 3A4 and resid 266 and name O)	(segid 3A4 and resid 270 and name O)	6.18	0.07	0.07
	assign (segid 3A4 and resid 266 and name O)	(segid 3A4 and resid 271 and name C)	7.22	0.12	0.11
	assign (segid 3A4 and resid 266 and name O)	(segid 3A4 and resid 271 and name CA)	6.38	0.11	0.11
	assign (segid 3A4 and resid 266 and name O)	(segid 3A4 and resid 271 and name CB)	6.56	0.15	0.14
80	assign (segid 3A4 and resid 266 and name O)	(segid 3A4 and resid 271 and name N)	5.03	0.10	0.10
	assign (segid 3A4 and resid 266 and name O)	(segid 3A4 and resid 272 and name N)	6.82	0.13	0.14
	assign (segid 3A4 and resid 266 and name O)	(segid 3A4 and resid 273 and name N)	7.73	0.16	0.15

	assign (segid 3A4 and resid 266 and name O)	(segid 3A4 and resid 312 and name CA)	7.18	0.34	0.34
	assign (segid 3A4 and resid 266 and name O)	(segid 3A4 and resid 312 and name CB)	6.18	0.25	0.25
	assign (segid 3A4 and resid 267 and name C)	(segid 3A4 and resid 267 and name CB)	2.54	0.01	0.01
	assign (segid 3A4 and resid 267 and name C)	(segid 3A4 and resid 267 and name O)	1.24	0.01	0.01
5	assign (segid 3A4 and resid 267 and name C)	(segid 3A4 and resid 268 and name C)	2.98	0.04	0.04
	assign (segid 3A4 and resid 267 and name C)	(segid 3A4 and resid 268 and name CA)	2.43	0.01	0.02
	assign (segid 3A4 and resid 267 and name C)	(segid 3A4 and resid 268 and name CB)	3.71	0.03	0.02
	assign (segid 3A4 and resid 267 and name C)	(segid 3A4 and resid 268 and name N)	1.33	0.01	0.00
	assign (segid 3A4 and resid 267 and name C)	(segid 3A4 and resid 268 and name O)	3.79	0.08	0.08
10	assign (segid 3A4 and resid 267 and name C)	(segid 3A4 and resid 269 and name C)	4.52	0.09	0.09
	assign (segid 3A4 and resid 267 and name C)	(segid 3A4 and resid 269 and name CA)	4.44	0.06	0.07
	assign (segid 3A4 and resid 267 and name C)	(segid 3A4 and resid 269 and name N)	3.28	0.05	0.05
	assign (segid 3A4 and resid 267 and name C)	(segid 3A4 and resid 269 and name O)	5.58	0.08	0.09
	assign (segid 3A4 and resid 267 and name C)	(segid 3A4 and resid 270 and name C)	4.83	0.10	0.11
	assign (segid 3A4 and resid 267 and name C)	(segid 3A4 and resid 270 and name CA)	4.61	0.13	0.13
15	assign (segid 3A4 and resid 267 and name C)	(segid 3A4 and resid 270 and name CB)	4.55	0.17	0.16
	assign (segid 3A4 and resid 267 and name C)	(segid 3A4 and resid 270 and name CD1)	5.62	0.21	0.22
	assign (segid 3A4 and resid 267 and name C)	(segid 3A4 and resid 270 and name CD2)	6.62	0.14	0.15
	assign (segid 3A4 and resid 267 and name C)	(segid 3A4 and resid 270 and name CG)	5.25	0.16	0.16
20	assign (segid 3A4 and resid 267 and name C)	(segid 3A4 and resid 270 and name N)	3.85	0.14	0.13
	assign (segid 3A4 and resid 267 and name C)	(segid 3A4 and resid 270 and name O)	6.03	0.11	0.11
	assign (segid 3A4 and resid 267 and name C)	(segid 3A4 and resid 271 and name C)	5.98	0.08	0.08
	assign (segid 3A4 and resid 267 and name C)	(segid 3A4 and resid 271 and name CA)	4.92	0.08	0.07
	assign (segid 3A4 and resid 267 and name C)	(segid 3A4 and resid 271 and name CB)	4.44	0.08	0.08
25	assign (segid 3A4 and resid 267 and name C)	(segid 3A4 and resid 271 and name N)	4.07	0.09	0.08
	assign (segid 3A4 and resid 267 and name C)	(segid 3A4 and resid 271 and name O)	7.14	0.08	0.08
	assign (segid 3A4 and resid 267 and name C)	(segid 3A4 and resid 272 and name CA)	7.12	0.13	0.13
	assign (segid 3A4 and resid 267 and name C)	(segid 3A4 and resid 272 and name CB)	7.14	0.17	0.17
	assign (segid 3A4 and resid 267 and name C)	(segid 3A4 and resid 272 and name N)	5.86	0.11	0.11
30	assign (segid 3A4 and resid 267 and name C)	(segid 3A4 and resid 272 and name O)	7.74	0.14	0.14
	assign (segid 3A4 and resid 267 and name CA)	(segid 3A4 and resid 273 and name N)	1.52	0.01	0.01
	assign (segid 3A4 and resid 267 and name CA)	(segid 3A4 and resid 267 and name C)	1.54	0.01	0.01
	assign (segid 3A4 and resid 267 and name CA)	(segid 3A4 and resid 267 and name CB)	2.39	0.01	0.01
	assign (segid 3A4 and resid 267 and name CA)	(segid 3A4 and resid 268 and name C)	4.37	0.05	0.04
35	assign (segid 3A4 and resid 267 and name CA)	(segid 3A4 and resid 268 and name CA)	3.82	0.01	0.01
	assign (segid 3A4 and resid 267 and name CA)	(segid 3A4 and resid 268 and name CB)	4.88	0.03	0.02
	assign (segid 3A4 and resid 267 and name CA)	(segid 3A4 and resid 268 and name N)	2.45	0.02	0.02
	assign (segid 3A4 and resid 267 and name CA)	(segid 3A4 and resid 268 and name O)	5.24	0.10	0.09
	assign (segid 3A4 and resid 267 and name CA)	(segid 3A4 and resid 269 and name C)	5.42	0.12	0.11
40	assign (segid 3A4 and resid 267 and name CA)	(segid 3A4 and resid 269 and name CA)	5.41	0.08	0.07
	assign (segid 3A4 and resid 267 and name CA)	(segid 3A4 and resid 269 and name N)	4.36	0.05	0.06
	assign (segid 3A4 and resid 267 and name CA)	(segid 3A4 and resid 269 and name O)	6.54	0.12	0.11
	assign (segid 3A4 and resid 267 and name CA)	(segid 3A4 and resid 270 and name C)	5.60	0.15	0.15
	assign (segid 3A4 and resid 267 and name CA)	(segid 3A4 and resid 270 and name CA)	5.13	0.16	0.15
	assign (segid 3A4 and resid 267 and name CA)	(segid 3A4 and resid 270 and name CB)	4.62	0.17	0.17
45	assign (segid 3A4 and resid 267 and name CA)	(segid 3A4 and resid 270 and name CD1)	5.00	0.23	0.23
	assign (segid 3A4 and resid 267 and name CA)	(segid 3A4 and resid 270 and name CD2)	6.48	0.18	0.18
	assign (segid 3A4 and resid 267 and name CA)	(segid 3A4 and resid 270 and name CG)	5.01	0.18	0.17
	assign (segid 3A4 and resid 267 and name CA)	(segid 3A4 and resid 270 and name N)	4.51	0.14	0.14
50	assign (segid 3A4 and resid 267 and name CA)	(segid 3A4 and resid 270 and name O)	6.76	0.16	0.16
	assign (segid 3A4 and resid 267 and name CA)	(segid 3A4 and resid 271 and name C)	7.21	0.12	0.11
	assign (segid 3A4 and resid 267 and name CA)	(segid 3A4 and resid 271 and name CA)	6.02	0.13	0.12
	assign (segid 3A4 and resid 267 and name CA)	(segid 3A4 and resid 271 and name CB)	5.64	0.13	0.13
	assign (segid 3A4 and resid 267 and name CA)	(segid 3A4 and resid 271 and name N)	5.07	0.13	0.13
	assign (segid 3A4 and resid 267 and name CA)	(segid 3A4 and resid 272 and name CA)	8.46	0.12	0.13
55	assign (segid 3A4 and resid 267 and name CA)	(segid 3A4 and resid 272 and name CB)	8.53	0.16	0.17
	assign (segid 3A4 and resid 267 and name CA)	(segid 3A4 and resid 272 and name N)	7.16	0.11	0.12
	assign (segid 3A4 and resid 267 and name CA)	(segid 3A4 and resid 273 and name CA)	9.81	0.17	0.16
	assign (segid 3A4 and resid 267 and name CA)	(segid 3A4 and resid 273 and name CB)	9.80	0.20	0.21
60	assign (segid 3A4 and resid 267 and name CA)	(segid 3A4 and resid 274 and name CA)	10.83	0.51	0.52
	assign (segid 3A4 and resid 267 and name CA)	(segid 3A4 and resid 274 and name CB)	11.79	0.71	0.70
	assign (segid 3A4 and resid 267 and name CA)	(segid 3A4 and resid 275 and name CA)	13.27	0.32	0.31
	assign (segid 3A4 and resid 267 and name CA)	(segid 3A4 and resid 275 and name CB)	14.26	0.28	0.28
	assign (segid 3A4 and resid 267 and name CA)	(segid 3A4 and resid 276 and name CA)	11.02	0.26	0.25
65	assign (segid 3A4 and resid 267 and name CA)	(segid 3A4 and resid 276 and name CB)	10.16	0.28	0.27
	assign (segid 3A4 and resid 267 and name CA)	(segid 3A4 and resid 277 and name CA)	9.34	0.32	0.33
	assign (segid 3A4 and resid 267 and name CA)	(segid 3A4 and resid 277 and name CB)	8.77	0.41	0.41
	assign (segid 3A4 and resid 267 and name CA)	(segid 3A4 and resid 278 and name CA)	12.98	0.37	0.37
	assign (segid 3A4 and resid 267 and name CA)	(segid 3A4 and resid 278 and name CB)	13.97	0.39	0.39
70	assign (segid 3A4 and resid 267 and name CA)	(segid 3A4 and resid 279 and name CA)	14.24	0.32	0.31
	assign (segid 3A4 and resid 267 and name CA)	(segid 3A4 and resid 279 and name CB)	14.24	0.25	0.26
	assign (segid 3A4 and resid 267 and name CA)	(segid 3A4 and resid 280 and name CA)	12.13	0.58	0.58
	assign (segid 3A4 and resid 267 and name CA)	(segid 3A4 and resid 280 and name CB)	10.67	0.60	0.61
	assign (segid 3A4 and resid 267 and name CA)	(segid 3A4 and resid 281 and name CA)	13.24	0.80	0.80
75	assign (segid 3A4 and resid 267 and name CA)	(segid 3A4 and resid 281 and name CB)	13.08	0.75	0.75
	assign (segid 3A4 and resid 267 and name CA)	(segid 3A4 and resid 282 and name CA)	16.71	0.73	0.73
	assign (segid 3A4 and resid 267 and name CA)	(segid 3A4 and resid 303 and name CA)	17.82	0.86	0.85
	assign (segid 3A4 and resid 267 and name CA)	(segid 3A4 and resid 304 and name CA)	15.35	0.80	0.81
	assign (segid 3A4 and resid 267 and name CA)	(segid 3A4 and resid 304 and name CB)	15.19	0.81	0.81
80	assign (segid 3A4 and resid 267 and name CA)	(segid 3A4 and resid 305 and name CA)	12.64	0.82	0.82
	assign (segid 3A4 and resid 267 and name CA)	(segid 3A4 and resid 305 and name CB)	12.67	0.79	0.79
	assign (segid 3A4 and resid 267 and name CA)	(segid 3A4 and resid 306 and name CA)	14.51	0.73	0.73
	assign (segid 3A4 and resid 267 and name CA)	(segid 3A4 and resid 307 and name CA)	14.70	0.80	0.80

	assign (segid 3A4 and resid 267 and name CA) (segid 3A4 and resid 307 and name CB)	15.43	0.85	0.85
	assign (segid 3A4 and resid 267 and name CA) (segid 3A4 and resid 308 and name CA)	11.02	0.84	0.85
	assign (segid 3A4 and resid 267 and name CA) (segid 3A4 and resid 308 and name CB)	10.21	0.91	0.91
	assign (segid 3A4 and resid 267 and name CA) (segid 3A4 and resid 309 and name CA)	10.73	0.62	0.62
5	assign (segid 3A4 and resid 267 and name CA) (segid 3A4 and resid 309 and name CB)	11.39	0.67	0.67
	assign (segid 3A4 and resid 267 and name CA) (segid 3A4 and resid 310 and name CA)	13.75	0.52	0.51
	assign (segid 3A4 and resid 267 and name CA) (segid 3A4 and resid 310 and name CB)	15.03	0.55	0.55
	assign (segid 3A4 and resid 267 and name CA) (segid 3A4 and resid 311 and name CA)	12.62	0.61	0.61
	assign (segid 3A4 and resid 267 and name CA) (segid 3A4 and resid 311 and name CB)	12.52	0.69	0.70
10	assign (segid 3A4 and resid 267 and name CA) (segid 3A4 and resid 312 and name CA)	9.54	0.50	0.49
	assign (segid 3A4 and resid 267 and name CA) (segid 3A4 and resid 312 and name CB)	8.40	0.41	0.42
	assign (segid 3A4 and resid 267 and name CA) (segid 3A4 and resid 313 and name CA)	12.23	0.32	0.32
	assign (segid 3A4 and resid 267 and name CA) (segid 3A4 and resid 313 and name CB)	13.08	0.28	0.28
	assign (segid 3A4 and resid 267 and name CA) (segid 3A4 and resid 314 and name CA)	14.59	0.42	0.43
15	assign (segid 3A4 and resid 267 and name CA) (segid 3A4 and resid 314 and name CB)	15.18	0.47	0.48
	assign (segid 3A4 and resid 267 and name CA) (segid 3A4 and resid 315 and name CA)	12.84	0.56	0.56
	assign (segid 3A4 and resid 267 and name CA) (segid 3A4 and resid 315 and name CB)	11.88	0.60	0.60
	assign (segid 3A4 and resid 267 and name CA) (segid 3A4 and resid 316 and name CA)	11.62	0.65	0.65
	assign (segid 3A4 and resid 267 and name CA) (segid 3A4 and resid 316 and name CB)	14.46	0.50	0.51
20	assign (segid 3A4 and resid 267 and name CA) (segid 3A4 and resid 317 and name CA)	14.24	0.25	0.26
	assign (segid 3A4 and resid 267 and name CA) (segid 3A4 and resid 318 and name CA)	13.42	0.35	0.36
	assign (segid 3A4 and resid 267 and name CA) (segid 3A4 and resid 318 and name CB)	17.94	0.26	0.26
	assign (segid 3A4 and resid 267 and name CA) (segid 3A4 and resid 319 and name CA)	18.51	0.30	0.30
	assign (segid 3A4 and resid 267 and name CA) (segid 3A4 and resid 319 and name CB)	19.08	0.61	0.61
25	assign (segid 3A4 and resid 267 and name CA) (segid 3A4 and resid 320 and name CA)	17.08	0.77	0.77
	assign (segid 3A4 and resid 267 and name CA) (segid 3A4 and resid 321 and name CA)	17.84	0.88	0.88
	assign (segid 3A4 and resid 267 and name CA) (segid 3A4 and resid 321 and name CB)	15.69	0.77	0.76
	assign (segid 3A4 and resid 267 and name CA) (segid 3A4 and resid 322 and name CA)	16.74	0.85	0.85
	assign (segid 3A4 and resid 267 and name CA) (segid 3A4 and resid 322 and name CB)	12.52	0.79	0.78
30	assign (segid 3A4 and resid 267 and name CA) (segid 3A4 and resid 323 and name CA)	11.11	0.77	0.76
	assign (segid 3A4 and resid 267 and name CA) (segid 3A4 and resid 323 and name CB)	14.29	0.81	0.82
	assign (segid 3A4 and resid 267 and name CA) (segid 3A4 and resid 324 and name CA)	15.76	0.81	0.80
	assign (segid 3A4 and resid 267 and name CA) (segid 3A4 and resid 324 and name CB)	13.64	0.89	0.89
	assign (segid 3A4 and resid 267 and name CA) (segid 3A4 and resid 325 and name CA)	12.83	0.95	0.95
35	assign (segid 3A4 and resid 267 and name CA) (segid 3A4 and resid 325 and name CB)	17.85	0.30	0.29
	assign (segid 3A4 and resid 267 and name CA) (segid 3A4 and resid 326 and name CA)	19.04	0.46	0.45
	assign (segid 3A4 and resid 267 and name CA) (segid 3A4 and resid 326 and name CB)	15.80	0.45	0.45
	assign (segid 3A4 and resid 267 and name CA) (segid 3A4 and resid 327 and name CA)	15.87	0.43	0.43
	assign (segid 3A4 and resid 267 and name CA) (segid 3A4 and resid 327 and name CB)	15.17	0.47	0.47
40	assign (segid 3A4 and resid 267 and name CA) (segid 3A4 and resid 328 and name CA)	16.14	0.52	0.53
	assign (segid 3A4 and resid 267 and name CA) (segid 3A4 and resid 328 and name CB)	16.24	0.45	0.45
	assign (segid 3A4 and resid 267 and name CA) (segid 3A4 and resid 329 and name CA)	17.59	0.46	0.47
	assign (segid 3A4 and resid 267 and name CA) (segid 3A4 and resid 329 and name CB)	14.04	0.64	0.63
	assign (segid 3A4 and resid 267 and name CA) (segid 3A4 and resid 330 and name CA)	14.21	0.71	0.71
45	assign (segid 3A4 and resid 267 and name CA) (segid 3A4 and resid 330 and name CB)	10.88	0.50	0.49
	assign (segid 3A4 and resid 267 and name CA) (segid 3A4 and resid 331 and name CA)	12.29	0.50	0.51
	assign (segid 3A4 and resid 267 and name CA) (segid 3A4 and resid 331 and name CB)	13.67	0.49	0.49
	assign (segid 3A4 and resid 267 and name CA) (segid 3A4 and resid 332 and name CA)	13.52	0.59	0.60
	assign (segid 3A4 and resid 267 and name CA) (segid 3A4 and resid 332 and name CB)	14.59	0.64	0.64
50	assign (segid 3A4 and resid 267 and name CA) (segid 3A4 and resid 333 and name CA)	10.54	0.73	0.74
	assign (segid 3A4 and resid 267 and name CA) (segid 3A4 and resid 333 and name CB)	9.88	0.80	0.80
	assign (segid 3A4 and resid 267 and name CA) (segid 3A4 and resid 334 and name CA)	8.44	0.70	0.71
	assign (segid 3A4 and resid 267 and name CA) (segid 3A4 and resid 334 and name CB)	8.08	0.71	0.72
	assign (segid 3A4 and resid 267 and name CA) (segid 3A4 and resid 335 and name CA)	11.71	0.84	0.84
55	assign (segid 3A4 and resid 267 and name CA) (segid 3A4 and resid 335 and name CB)	12.52	0.67	0.66
	assign (segid 3A4 and resid 267 and name CA) (segid 3A4 and resid 336 and name CA)	13.13	0.63	0.62
	assign (segid 3A4 and resid 267 and name CA) (segid 3A4 and resid 336 and name CB)	9.62	0.60	0.60
	assign (segid 3A4 and resid 267 and name CA) (segid 3A4 and resid 337 and name CA)	8.21	0.62	0.63
	assign (segid 3A4 and resid 267 and name CA) (segid 3A4 and resid 337 and name CB)	9.79	0.51	0.52
60	assign (segid 3A4 and resid 267 and name CA) (segid 3A4 and resid 338 and name CA)	9.43	0.64	0.64
	assign (segid 3A4 and resid 267 and name CA) (segid 3A4 and resid 338 and name CB)	13.46	0.50	0.50
	assign (segid 3A4 and resid 267 and name CA) (segid 3A4 and resid 339 and name CA)	13.81	0.26	0.26
	assign (segid 3A4 and resid 267 and name CA) (segid 3A4 and resid 339 and name CB)	13.75	0.39	0.38
	assign (segid 3A4 and resid 267 and name CA) (segid 3A4 and resid 340 and name CA)	11.82	0.18	0.19
65	assign (segid 3A4 and resid 267 and name CA) (segid 3A4 and resid 340 and name CB)	11.45	0.89	0.89
	assign (segid 3A4 and resid 267 and name CA) (segid 3A4 and resid 341 and name CA)	8.96	0.61	0.61
	assign (segid 3A4 and resid 267 and name CA) (segid 3A4 and resid 341 and name CB)	9.50	0.66	0.66
	assign (segid 3A4 and resid 267 and name CA) (segid 3A4 and resid 342 and name CA)	10.65	0.83	0.83
	assign (segid 3A4 and resid 267 and name CA) (segid 3A4 and resid 342 and name CB)	9.89	1.22	1.23
70	assign (segid 3A4 and resid 267 and name CA) (segid 3A4 and resid 343 and name CA)	13.25	1.12	1.12
	assign (segid 3A4 and resid 267 and name CA) (segid 3A4 and resid 343 and name CB)	13.53	1.01	1.02
	assign (segid 3A4 and resid 267 and name CA) (segid 3A4 and resid 344 and name CA)	12.08	1.31	1.31
	assign (segid 3A4 and resid 267 and name CA) (segid 3A4 and resid 344 and name CB)	13.02	0.69	0.68
	assign (segid 3A4 and resid 267 and name CA) (segid 3A4 and resid 345 and name CA)	13.75	0.40	0.40
75	assign (segid 3A4 and resid 267 and name CA) (segid 3A4 and resid 345 and name CB)	15.28	1.02	1.01
	assign (segid 3A4 and resid 267 and name CA) (segid 3A4 and resid 346 and name CA)	18.04	1.16	1.15
	assign (segid 3A4 and resid 267 and name CA) (segid 3A4 and resid 346 and name CB)	14.81	0.48	0.48
80	assign (segid 3A4 and resid 267 and name CA) (segid 3A4 and resid 347 and name CA)	12.05	0.46	0.46
	assign (segid 3A4 and resid 267 and name CA) (segid 3A4 and resid 347 and name CB)	10.33	0.14	0.14
	assign (segid 3A4 and resid 267 and name CA) (segid 3A4 and resid 348 and name CA)	12.61	0.44	0.44
	assign (segid 3A4 and resid 267 and name CA) (segid 3A4 and resid 348 and name CB)	11.76	0.50	0.50
	assign (segid 3A4 and resid 267 and name CA) (segid 3A4 and resid 349 and name CA)	8.95	0.44	0.44
	assign (segid 3A4 and resid 267 and name CA) (segid 3A4 and resid 349 and name CB)	10.48	0.22	0.22

	assign (segid 3A4 and resid 267 and name CA)	(segid 3A4 and resid 440 and name CA)	9.30	0.25	0.26
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 268 and name C)	5.46	0.04	0.04
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 268 and name CA)	4.57	0.08	0.08
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 268 and name CB)	5.47	0.10	0.11
5	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 268 and name N)	3.23	0.06	0.07
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 268 and name O)	6.28	0.08	0.07
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 269 and name C)	6.86	0.12	0.11
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 269 and name CA)	6.82	0.06	0.06
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 269 and name N)	5.67	0.07	0.06
10	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 270 and name C)	6.73	0.19	0.20
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 270 and name CA)	6.45	0.21	0.20
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 270 and name CB)	5.83	0.23	0.23
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 270 and name CD1)	6.02	0.23	0.23
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 270 and name CG)	6.27	0.22	0.21
15	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 270 and name N)	5.95	0.16	0.17
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 271 and name CA)	6.78	0.14	0.13
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 271 and name CB)	6.14	0.13	0.14
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 271 and name N)	6.07	0.16	0.15
20	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 272 and name CA)	9.51	0.13	0.13
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 272 and name CB)	9.62	0.17	0.18
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 273 and name CA)	11.08	0.18	0.18
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 273 and name CB)	11.19	0.22	0.22
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 274 and name CA)	11.86	0.53	0.52
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 274 and name CB)	12.71	0.74	0.74
25	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 275 and name CA)	14.46	0.34	0.33
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 275 and name CB)	15.51	0.30	0.31
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 276 and name CA)	12.32	0.28	0.28
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 276 and name CB)	11.54	0.31	0.30
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 277 and name CA)	10.33	0.30	0.30
30	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 277 and name CB)	9.67	0.37	0.36
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 278 and name CA)	13.85	0.35	0.36
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 278 and name CB)	14.87	0.39	0.38
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 279 and name CA)	15.28	0.30	0.30
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 279 and name CB)	15.39	0.23	0.23
35	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 280 and name CA)	13.02	0.54	0.54
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 280 and name CB)	11.57	0.54	0.54
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 281 and name CA)	13.80	0.78	0.78
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 281 and name CB)	13.59	0.74	0.74
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 282 and name CA)	17.39	0.73	0.73
40	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 304 and name CA)	16.35	0.78	0.78
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 304 and name CB)	16.23	0.79	0.79
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 305 and name CA)	13.46	0.81	0.80
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 305 and name CB)	13.32	0.80	0.80
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 306 and name CA)	15.33	0.71	0.71
45	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 307 and name CA)	15.81	0.76	0.76
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 307 and name CB)	16.60	0.81	0.80
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 308 and name CA)	12.21	0.81	0.80
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 308 and name CB)	11.35	0.86	0.86
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 309 and name CA)	11.63	0.59	0.60
50	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 309 and name CB)	12.15	0.64	0.63
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 310 and name CA)	14.78	0.51	0.51
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 310 and name CB)	16.08	0.53	0.54
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 311 and name CA)	13.89	0.61	0.61
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 311 and name CB)	13.87	0.68	0.69
55	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 312 and name CA)	10.69	0.54	0.55
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 312 and name CB)	9.49	0.47	0.48
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 313 and name CA)	13.13	0.39	0.39
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 313 and name CB)	13.91	0.34	0.33
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 314 and name CA)	15.71	0.48	0.47
60	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 314 and name CB)	16.38	0.51	0.51
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 315 and name CA)	14.04	0.59	0.60
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 315 and name CB)	13.16	0.63	0.63
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 316 and name CA)	12.52	0.66	0.67
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 317 and name CA)	15.21	0.55	0.54
65	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 318 and name CA)	14.63	0.35	0.35
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 318 and name CB)	13.73	0.44	0.43
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 319 and name CA)	18.28	0.33	0.33
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 319 and name CB)	18.82	0.34	0.35
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 361 and name CA)	18.45	0.77	0.76
70	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 362 and name CA)	17.16	0.77	0.77
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 362 and name CB)	18.23	0.84	0.85
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 363 and name CA)	14.01	0.78	0.79
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 363 and name CB)	12.60	0.76	0.76
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 364 and name CA)	15.81	0.78	0.78
75	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 364 and name CB)	17.27	0.78	0.78
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 365 and name CA)	15.05	0.85	0.85
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 365 and name CB)	14.20	0.91	0.92
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 383 and name CA)	18.57	0.35	0.34
80	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 396 and name CA)	18.95	0.54	0.53
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 397 and name CA)	15.80	0.53	0.52
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 397 and name CB)	15.94	0.51	0.50
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 398 and name CA)	15.43	0.54	0.55
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 398 and name CB)	16.51	0.59	0.60

	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 399 and name CA)	16.27	0.53	0.52
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 399 and name CB)	17.55	0.53	0.54
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 100 and name CA)	13.78	0.70	0.69
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 400 and name CB)	13.87	0.75	0.75
5	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 401 and name CA)	10.89	0.54	0.54
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 402 and name CA)	12.50	0.55	0.56
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 402 and name CB)	13.94	0.54	0.55
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 403 and name CA)	13.34	0.66	0.66
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 403 and name CB)	14.31	0.71	0.72
10	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 404 and name CA)	10.09	0.78	0.77
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 404 and name CB)	9.37	0.83	0.82
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 405 and name CA)	8.43	0.72	0.73
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 405 and name CB)	8.32	0.68	0.69
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 406 and name CA)	11.76	0.82	0.82
15	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 407 and name CA)	12.11	0.68	0.68
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 407 and name CB)	12.60	0.65	0.65
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 408 and name CA)	9.03	0.64	0.64
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 408 and name CB)	7.58	0.66	0.65
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 409 and name CA)	9.69	0.51	0.52
20	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 409 and name CB)	9.56	0.61	0.61
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 410 and name CA)	13.28	0.48	0.47
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 411 and name CA)	13.25	0.23	0.23
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 411 and name CB)	13.06	0.35	0.34
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 412 and name CA)	11.29	0.19	0.20
25	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 413 and name CA)	11.25	0.86	0.86
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 414 and name CA)	8.68	0.63	0.63
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 415 and name CA)	9.29	0.64	0.65
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 415 and name CB)	10.49	0.70	0.70
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 416 and name CA)	9.59	1.30	1.31
30	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 417 and name CA)	12.81	1.31	1.31
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 423 and name CA)	13.52	0.97	0.98
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 424 and name CA)	12.15	1.40	1.39
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 425 and name CA)	13.02	0.68	0.68
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 426 and name CA)	13.79	0.55	0.56
35	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 427 and name CA)	15.25	0.94	0.94
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 428 and name CA)	18.00	1.12	1.11
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 433 and name CA)	14.95	0.44	0.44
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 434 and name CA)	11.98	0.53	0.53
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 435 and name CA)	10.10	0.30	0.30
40	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 436 and name CA)	12.05	0.44	0.44
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 437 and name CA)	10.94	0.57	0.57
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 438 and name CA)	8.12	0.53	0.53
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 439 and name CA)	9.49	0.23	0.23
	assign (segid 3A4 and resid 267 and name CB)	(segid 3A4 and resid 440 and name CA)	8.36	0.23	0.24
45	assign (segid 3A4 and resid 267 and name N)	(segid 3A4 and resid 267 and name C)	2.47	0.02	0.01
	assign (segid 3A4 and resid 267 and name N)	(segid 3A4 and resid 267 and name CA)	1.46	0.01	0.02
	assign (segid 3A4 and resid 267 and name N)	(segid 3A4 and resid 267 and name CB)	2.46	0.02	0.03
	assign (segid 3A4 and resid 267 and name N)	(segid 3A4 and resid 267 and name O)	3.51	0.03	0.03
	assign (segid 3A4 and resid 267 and name N)	(segid 3A4 and resid 268 and name C)	4.69	0.02	0.03
50	assign (segid 3A4 and resid 267 and name N)	(segid 3A4 and resid 268 and name CA)	4.23	0.02	0.02
	assign (segid 3A4 and resid 267 and name N)	(segid 3A4 and resid 268 and name CB)	4.97	0.04	0.04
	assign (segid 3A4 and resid 267 and name N)	(segid 3A4 and resid 268 and name N)	2.84	0.03	0.03
	assign (segid 3A4 and resid 267 and name N)	(segid 3A4 and resid 268 and name O)	5.75	0.05	0.05
	assign (segid 3A4 and resid 267 and name N)	(segid 3A4 and resid 269 and name C)	5.58	0.07	0.08
55	assign (segid 3A4 and resid 267 and name N)	(segid 3A4 and resid 269 and name CA)	5.32	0.09	0.08
	assign (segid 3A4 and resid 267 and name N)	(segid 3A4 and resid 269 and name N)	4.33	0.06	0.06
	assign (segid 3A4 and resid 267 and name N)	(segid 3A4 and resid 269 and name O)	6.79	0.07	0.07
	assign (segid 3A4 and resid 267 and name N)	(segid 3A4 and resid 270 and name C)	6.40	0.10	0.11
60	assign (segid 3A4 and resid 267 and name N)	(segid 3A4 and resid 270 and name CA)	5.64	0.10	0.10
	assign (segid 3A4 and resid 267 and name N)	(segid 3A4 and resid 270 and name CB)	5.18	0.12	0.12
	assign (segid 3A4 and resid 267 and name N)	(segid 3A4 and resid 270 and name CD1)	5.18	0.22	0.22
	assign (segid 3A4 and resid 267 and name N)	(segid 3A4 and resid 270 and name CD2)	6.59	0.14	0.15
	assign (segid 3A4 and resid 267 and name N)	(segid 3A4 and resid 270 and name CG)	5.18	0.13	0.14
	assign (segid 3A4 and resid 267 and name N)	(segid 3A4 and resid 270 and name N)	4.80	0.09	0.09
65	assign (segid 3A4 and resid 267 and name N)	(segid 3A4 and resid 270 and name O)	7.59	0.11	0.11
	assign (segid 3A4 and resid 267 and name N)	(segid 3A4 and resid 271 and name CA)	7.11	0.09	0.09
	assign (segid 3A4 and resid 267 and name N)	(segid 3A4 and resid 271 and name CB)	6.83	0.10	0.10
	assign (segid 3A4 and resid 267 and name N)	(segid 3A4 and resid 271 and name N)	6.02	0.09	0.09
	assign (segid 3A4 and resid 267 and name N)	(segid 3A4 and resid 312 and name CB)	7.12	0.45	0.46
70	assign (segid 3A4 and resid 267 and name O)	(segid 3A4 and resid 267 and name CB)	3.32	0.03	0.02
	assign (segid 3A4 and resid 267 and name O)	(segid 3A4 and resid 268 and name C)	2.90	0.08	0.08
	assign (segid 3A4 and resid 267 and name O)	(segid 3A4 and resid 268 and name CA)	2.75	0.03	0.02
	assign (segid 3A4 and resid 267 and name O)	(segid 3A4 and resid 268 and name CB)	4.23	0.03	0.03
	assign (segid 3A4 and resid 267 and name O)	(segid 3A4 and resid 268 and name N)	2.24	0.02	0.01
75	assign (segid 3A4 and resid 267 and name O)	(segid 3A4 and resid 268 and name O)	3.32	0.13	0.13
	assign (segid 3A4 and resid 267 and name O)	(segid 3A4 and resid 269 and name C)	4.07	0.15	0.14
	assign (segid 3A4 and resid 267 and name O)	(segid 3A4 and resid 269 and name CA)	4.34	0.12	0.11
	assign (segid 3A4 and resid 267 and name O)	(segid 3A4 and resid 269 and name N)	3.40	0.09	0.10
80	assign (segid 3A4 and resid 267 and name O)	(segid 3A4 and resid 269 and name O)	4.96	0.12	0.13
	assign (segid 3A4 and resid 267 and name O)	(segid 3A4 and resid 270 and name C)	3.78	0.13	0.13
	assign (segid 3A4 and resid 267 and name O)	(segid 3A4 and resid 270 and name CA)	3.85	0.19	0.19
	assign (segid 3A4 and resid 267 and name O)	(segid 3A4 and resid 270 and name CB)	3.89	0.20	0.21
	assign (segid 3A4 and resid 267 and name O)	(segid 3A4 and resid 270 and name CD1)	5.41	0.23	0.23

	assign (segid 3A4 and resid 267 and name O) (segid 3A4 and resid 270 and name CD2)	6.19	0.19	0.18
	assign (segid 3A4 and resid 267 and name O) (segid 3A4 and resid 270 and name CG)	4.90	0.20	0.20
	assign (segid 3A4 and resid 267 and name O) (segid 3A4 and resid 270 and name N)	3.34	0.21	0.20
	assign (segid 3A4 and resid 267 and name O) (segid 3A4 and resid 270 and name O)	4.94	0.12	0.11
5	assign (segid 3A4 and resid 267 and name O) (segid 3A4 and resid 271 and name C)	4.86	0.10	0.10
	assign (segid 3A4 and resid 267 and name O) (segid 3A4 and resid 271 and name CA)	3.72	0.09	0.09
	assign (segid 3A4 and resid 267 and name O) (segid 3A4 and resid 271 and name CB)	3.35	0.13	0.12
	assign (segid 3A4 and resid 267 and name O) (segid 3A4 and resid 271 and name N)	2.91	0.09	0.10
	assign (segid 3A4 and resid 267 and name O) (segid 3A4 and resid 271 and name O)	6.00	0.10	0.09
10	assign (segid 3A4 and resid 267 and name O) (segid 3A4 and resid 272 and name C)	7.12	0.16	0.16
	assign (segid 3A4 and resid 267 and name O) (segid 3A4 and resid 272 and name CA)	6.23	0.14	0.15
	assign (segid 3A4 and resid 267 and name O) (segid 3A4 and resid 272 and name CB)	6.46	0.19	0.18
	assign (segid 3A4 and resid 267 and name O) (segid 3A4 and resid 272 and name N)	4.88	0.13	0.13
	assign (segid 3A4 and resid 267 and name O) (segid 3A4 and resid 273 and name N)	6.80	0.16	0.16
15	assign (segid 3A4 and resid 267 and name O) (segid 3A4 and resid 268 and name CB)	2.50	0.02	0.01
	assign (segid 3A4 and resid 268 and name C) (segid 3A4 and resid 268 and name O)	1.24	0.01	0.01
	assign (segid 3A4 and resid 268 and name C) (segid 3A4 and resid 269 and name C)	3.06	0.05	0.04
	assign (segid 3A4 and resid 268 and name C) (segid 3A4 and resid 269 and name CA)	2.44	0.02	0.02
	assign (segid 3A4 and resid 268 and name C) (segid 3A4 and resid 269 and name N)	1.33	0.01	0.01
20	assign (segid 3A4 and resid 268 and name C) (segid 3A4 and resid 269 and name O)	3.88	0.04	0.04
	assign (segid 3A4 and resid 268 and name C) (segid 3A4 and resid 270 and name C)	4.57	0.09	0.08
	assign (segid 3A4 and resid 268 and name C) (segid 3A4 and resid 270 and name CA)	4.54	0.10	0.11
	assign (segid 3A4 and resid 268 and name C) (segid 3A4 and resid 270 and name CB)	5.37	0.13	0.13
	assign (segid 3A4 and resid 268 and name C) (segid 3A4 and resid 270 and name CD1)	7.14	0.17	0.17
25	assign (segid 3A4 and resid 268 and name C) (segid 3A4 and resid 270 and name CD2)	7.13	0.08	0.08
	assign (segid 3A4 and resid 268 and name C) (segid 3A4 and resid 270 and name CG)	6.16	0.11	0.12
	assign (segid 3A4 and resid 268 and name C) (segid 3A4 and resid 270 and name N)	3.37	0.11	0.11
	assign (segid 3A4 and resid 268 and name C) (segid 3A4 and resid 270 and name O)	5.65	0.09	0.09
	assign (segid 3A4 and resid 268 and name C) (segid 3A4 and resid 271 and name C)	4.79	0.09	0.10
30	assign (segid 3A4 and resid 268 and name C) (segid 3A4 and resid 271 and name CA)	4.48	0.09	0.09
	assign (segid 3A4 and resid 268 and name C) (segid 3A4 and resid 271 and name CB)	4.23	0.13	0.13
	assign (segid 3A4 and resid 268 and name C) (segid 3A4 and resid 271 and name N)	3.77	0.11	0.10
	assign (segid 3A4 and resid 268 and name C) (segid 3A4 and resid 271 and name O)	5.98	0.10	0.11
	assign (segid 3A4 and resid 268 and name C) (segid 3A4 and resid 272 and name C)	5.99	0.13	0.13
35	assign (segid 3A4 and resid 268 and name C) (segid 3A4 and resid 272 and name CA)	4.96	0.17	0.17
	assign (segid 3A4 and resid 268 and name C) (segid 3A4 and resid 272 and name CB)	4.54	0.21	0.20
	assign (segid 3A4 and resid 268 and name C) (segid 3A4 and resid 272 and name N)	4.08	0.14	0.15
	assign (segid 3A4 and resid 268 and name C) (segid 3A4 and resid 272 and name O)	7.05	0.13	0.13
	assign (segid 3A4 and resid 268 and name C) (segid 3A4 and resid 273 and name CA)	7.23	0.15	0.15
40	assign (segid 3A4 and resid 268 and name C) (segid 3A4 and resid 273 and name CB)	7.24	0.18	0.18
	assign (segid 3A4 and resid 268 and name C) (segid 3A4 and resid 273 and name N)	6.00	0.17	0.17
	assign (segid 3A4 and resid 268 and name CA) (segid 3A4 and resid 268 and name C)	1.52	0.02	0.01
	assign (segid 3A4 and resid 268 and name CA) (segid 3A4 and resid 268 and name CB)	1.52	0.01	0.01
	assign (segid 3A4 and resid 268 and name CA) (segid 3A4 and resid 269 and name C)	2.40	0.01	0.01
45	assign (segid 3A4 and resid 268 and name CA) (segid 3A4 and resid 269 and name CA)	4.45	0.05	0.05
	assign (segid 3A4 and resid 268 and name CA) (segid 3A4 and resid 269 and name N)	3.81	0.02	0.03
	assign (segid 3A4 and resid 268 and name CA) (segid 3A4 and resid 269 and name O)	2.44	0.02	0.02
	assign (segid 3A4 and resid 268 and name CA) (segid 3A4 and resid 270 and name C)	5.34	0.04	0.04
50	assign (segid 3A4 and resid 268 and name CA) (segid 3A4 and resid 270 and name CA)	5.53	0.09	0.09
	assign (segid 3A4 and resid 268 and name CA) (segid 3A4 and resid 270 and name CB)	5.57	0.11	0.10
	assign (segid 3A4 and resid 268 and name CA) (segid 3A4 and resid 270 and name CD1)	6.09	0.14	0.15
	assign (segid 3A4 and resid 268 and name CA) (segid 3A4 and resid 270 and name CD2)	7.62	0.20	0.20
	assign (segid 3A4 and resid 268 and name CA) (segid 3A4 and resid 270 and name CG)	6.89	0.14	0.14
	assign (segid 3A4 and resid 268 and name CA) (segid 3A4 and resid 270 and name N)	4.48	0.12	0.12
55	assign (segid 3A4 and resid 268 and name CA) (segid 3A4 and resid 270 and name O)	6.66	0.08	0.08
	assign (segid 3A4 and resid 268 and name CA) (segid 3A4 and resid 271 and name C)	5.65	0.09	0.08
	assign (segid 3A4 and resid 268 and name CA) (segid 3A4 and resid 271 and name CA)	5.09	0.10	0.09
	assign (segid 3A4 and resid 268 and name CA) (segid 3A4 and resid 271 and name CB)	4.41	0.12	0.12
	assign (segid 3A4 and resid 268 and name CA) (segid 3A4 and resid 271 and name N)	4.55	0.09	0.10
60	assign (segid 3A4 and resid 268 and name CA) (segid 3A4 and resid 271 and name O)	6.79	0.09	0.09
	assign (segid 3A4 and resid 268 and name CA) (segid 3A4 and resid 272 and name C)	7.29	0.13	0.13
	assign (segid 3A4 and resid 268 and name CA) (segid 3A4 and resid 272 and name CA)	6.13	0.17	0.16
	assign (segid 3A4 and resid 268 and name CA) (segid 3A4 and resid 272 and name CB)	5.74	0.18	0.19
	assign (segid 3A4 and resid 268 and name CA) (segid 3A4 and resid 272 and name N)	5.17	0.14	0.14
65	assign (segid 3A4 and resid 268 and name CA) (segid 3A4 and resid 273 and name CA)	8.63	0.14	0.14
	assign (segid 3A4 and resid 268 and name CA) (segid 3A4 and resid 273 and name CB)	8.72	0.17	0.17
	assign (segid 3A4 and resid 268 and name CA) (segid 3A4 and resid 273 and name N)	7.36	0.16	0.16
	assign (segid 3A4 and resid 268 and name CA) (segid 3A4 and resid 274 and name CA)	10.58	0.44	0.44
	assign (segid 3A4 and resid 268 and name CA) (segid 3A4 and resid 274 and name CB)	11.32	0.58	0.59
70	assign (segid 3A4 and resid 268 and name CA) (segid 3A4 and resid 275 and name CA)	13.30	0.23	0.23
	assign (segid 3A4 and resid 268 and name CA) (segid 3A4 and resid 275 and name CB)	14.02	0.19	0.20
	assign (segid 3A4 and resid 268 and name CA) (segid 3A4 and resid 276 and name CA)	11.65	0.20	0.19
	assign (segid 3A4 and resid 268 and name CA) (segid 3A4 and resid 276 and name CB)	10.59	0.19	0.18
	assign (segid 3A4 and resid 268 and name CA) (segid 3A4 and resid 277 and name CA)	10.78	0.39	0.38
75	assign (segid 3A4 and resid 268 and name CA) (segid 3A4 and resid 277 and name CB)	10.05	0.49	0.49
	assign (segid 3A4 and resid 268 and name CA) (segid 3A4 and resid 278 and name CA)	14.37	0.39	0.38
	assign (segid 3A4 and resid 268 and name CA) (segid 3A4 and resid 278 and name CB)	15.04	0.40	0.39
	assign (segid 3A4 and resid 268 and name CA) (segid 3A4 and resid 279 and name CA)	15.80	0.32	0.32
	assign (segid 3A4 and resid 268 and name CA) (segid 3A4 and resid 279 and name CB)	15.58	0.29	0.30
80	assign (segid 3A4 and resid 268 and name CA) (segid 3A4 and resid 280 and name CA)	14.45	0.58	0.57
	assign (segid 3A4 and resid 268 and name CA) (segid 3A4 and resid 280 and name CB)	13.08	0.63	0.63
	assign (segid 3A4 and resid 268 and name CA) (segid 3A4 and resid 281 and name CA)	15.77	0.78	0.79
	assign (segid 3A4 and resid 268 and name CA) (segid 3A4 and resid 281 and name CB)	15.45	0.75	0.75

	assign (segid 3A4 and resid 268 and name CA)	(segid 3A4 and resid 304 and name CA)	17.65	0.78	0.78
	assign (segid 3A4 and resid 268 and name CA)	(segid 3A4 and resid 304 and name CB)	17.34	0.76	0.76
	assign (segid 3A4 and resid 268 and name CA)	(segid 3A4 and resid 305 and name CA)	15.41	0.79	0.79
	assign (segid 3A4 and resid 268 and name CA)	(segid 3A4 and resid 305 and name CB)	15.70	0.74	0.73
5	assign (segid 3A4 and resid 268 and name CA)	(segid 3A4 and resid 306 and name CA)	17.07	0.77	0.78
	assign (segid 3A4 and resid 268 and name CA)	(segid 3A4 and resid 307 and name CA)	16.54	0.89	0.90
	assign (segid 3A4 and resid 268 and name CA)	(segid 3A4 and resid 307 and name CB)	17.18	0.95	0.94
	assign (segid 3A4 and resid 268 and name CA)	(segid 3A4 and resid 308 and name CA)	12.82	0.92	0.92
	assign (segid 3A4 and resid 268 and name CA)	(segid 3A4 and resid 308 and name CB)	12.26	0.94	0.95
	assign (segid 3A4 and resid 268 and name CA)	(segid 3A4 and resid 309 and name CA)	12.85	0.75	0.76
10	assign (segid 3A4 and resid 268 and name CA)	(segid 3A4 and resid 309 and name CB)	13.81	0.78	0.78
	assign (segid 3A4 and resid 268 and name CA)	(segid 3A4 and resid 310 and name CA)	15.19	0.68	0.68
	assign (segid 3A4 and resid 268 and name CA)	(segid 3A4 and resid 310 and name CB)	16.49	0.70	0.71
	assign (segid 3A4 and resid 268 and name CA)	(segid 3A4 and resid 311 and name CA)	13.25	0.79	0.80
	assign (segid 3A4 and resid 268 and name CA)	(segid 3A4 and resid 311 and name CB)	13.10	0.87	0.88
15	assign (segid 3A4 and resid 268 and name CA)	(segid 3A4 and resid 312 and name CA)	10.16	0.65	0.65
	assign (segid 3A4 and resid 268 and name CA)	(segid 3A4 and resid 312 and name CB)	9.48	0.59	0.58
	assign (segid 3A4 and resid 268 and name CA)	(segid 3A4 and resid 313 and name CA)	12.90	0.46	0.46
	assign (segid 3A4 and resid 268 and name CA)	(segid 3A4 and resid 313 and name CB)	14.06	0.44	0.45
20	assign (segid 3A4 and resid 268 and name CA)	(segid 3A4 and resid 314 and name CA)	14.54	0.57	0.57
	assign (segid 3A4 and resid 268 and name CA)	(segid 3A4 and resid 314 and name CB)	15.15	0.66	0.66
	assign (segid 3A4 and resid 268 and name CA)	(segid 3A4 and resid 315 and name CA)	11.94	0.63	0.63
	assign (segid 3A4 and resid 268 and name CA)	(segid 3A4 and resid 315 and name CB)	10.93	0.70	0.70
	assign (segid 3A4 and resid 268 and name CA)	(segid 3A4 and resid 316 and name CA)	10.70	0.48	0.48
25	assign (segid 3A4 and resid 268 and name CA)	(segid 3A4 and resid 317 and name CA)	13.98	0.35	0.35
	assign (segid 3A4 and resid 268 and name CA)	(segid 3A4 and resid 318 and name CA)	13.91	0.20	0.21
	assign (segid 3A4 and resid 268 and name CA)	(segid 3A4 and resid 318 and name CB)	13.41	0.31	0.31
	assign (segid 3A4 and resid 268 and name CA)	(segid 3A4 and resid 319 and name CA)	17.68	0.17	0.16
	assign (segid 3A4 and resid 268 and name CA)	(segid 3A4 and resid 319 and name CB)	18.52	0.14	0.15
30	assign (segid 3A4 and resid 268 and name CA)	(segid 3A4 and resid 348 and name CA)	17.92	0.86	0.86
	assign (segid 3A4 and resid 268 and name CA)	(segid 3A4 and resid 351 and name CA)	18.80	0.55	0.55
	assign (segid 3A4 and resid 268 and name CA)	(segid 3A4 and resid 352 and name CA)	18.70	0.55	0.55
	assign (segid 3A4 and resid 268 and name CA)	(segid 3A4 and resid 352 and name CB)	18.07	0.64	0.64
	assign (segid 3A4 and resid 268 and name CA)	(segid 3A4 and resid 360 and name CA)	17.59	0.74	0.73
35	assign (segid 3A4 and resid 268 and name CA)	(segid 3A4 and resid 360 and name CB)	18.53	0.70	0.69
	assign (segid 3A4 and resid 268 and name CA)	(segid 3A4 and resid 361 and name CA)	15.02	0.86	0.85
	assign (segid 3A4 and resid 268 and name CA)	(segid 3A4 and resid 361 and name CB)	15.51	0.94	0.95
	assign (segid 3A4 and resid 268 and name CA)	(segid 3A4 and resid 362 and name CA)	13.97	0.93	0.94
	assign (segid 3A4 and resid 268 and name CA)	(segid 3A4 and resid 362 and name CB)	15.12	1.00	1.01
40	assign (segid 3A4 and resid 268 and name CA)	(segid 3A4 and resid 363 and name CA)	11.45	0.98	0.98
	assign (segid 3A4 and resid 268 and name CA)	(segid 3A4 and resid 363 and name CB)	9.96	0.96	0.97
	assign (segid 3A4 and resid 268 and name CA)	(segid 3A4 and resid 364 and name CA)	14.03	0.99	0.98
	assign (segid 3A4 and resid 268 and name CA)	(segid 3A4 and resid 364 and name CB)	15.33	0.99	1.00
	assign (segid 3A4 and resid 268 and name CA)	(segid 3A4 and resid 365 and name CA)	14.39	0.99	0.99
45	assign (segid 3A4 and resid 268 and name CA)	(segid 3A4 and resid 365 and name CB)	13.86	1.00	1.00
	assign (segid 3A4 and resid 268 and name CA)	(segid 3A4 and resid 383 and name CA)	18.28	0.38	0.38
	assign (segid 3A4 and resid 268 and name CA)	(segid 3A4 and resid 397 and name CA)	18.31	0.33	0.34
	assign (segid 3A4 and resid 268 and name CA)	(segid 3A4 and resid 397 and name CB)	18.13	0.32	0.32
	assign (segid 3A4 and resid 268 and name CA)	(segid 3A4 and resid 398 and name CA)	17.86	0.37	0.38
	assign (segid 3A4 and resid 268 and name CA)	(segid 3A4 and resid 398 and name CB)	18.75	0.45	0.44
50	assign (segid 3A4 and resid 268 and name CA)	(segid 3A4 and resid 400 and name CA)	17.30	0.57	0.57
	assign (segid 3A4 and resid 268 and name CA)	(segid 3A4 and resid 400 and name CB)	17.32	0.66	0.65
	assign (segid 3A4 and resid 268 and name CA)	(segid 3A4 and resid 401 and name CA)	14.05	0.42	0.43
	assign (segid 3A4 and resid 268 and name CA)	(segid 3A4 and resid 402 and name CA)	15.67	0.43	0.43
	assign (segid 3A4 and resid 268 and name CA)	(segid 3A4 and resid 402 and name CB)	16.96	0.41	0.42
55	assign (segid 3A4 and resid 268 and name CA)	(segid 3A4 and resid 403 and name CA)	17.21	0.53	0.53
	assign (segid 3A4 and resid 268 and name CA)	(segid 3A4 and resid 403 and name CB)	18.26	0.57	0.58
	assign (segid 3A4 and resid 268 and name CA)	(segid 3A4 and resid 404 and name CA)	14.28	0.70	0.69
	assign (segid 3A4 and resid 268 and name CA)	(segid 3A4 and resid 404 and name CB)	13.51	0.74	0.75
60	assign (segid 3A4 and resid 268 and name CA)	(segid 3A4 and resid 405 and name CA)	12.16	0.69	0.68
	assign (segid 3A4 and resid 268 and name CA)	(segid 3A4 and resid 405 and name CB)	11.65	0.69	0.69
	assign (segid 3A4 and resid 268 and name CA)	(segid 3A4 and resid 406 and name CA)	15.35	0.83	0.83
	assign (segid 3A4 and resid 268 and name CA)	(segid 3A4 and resid 407 and name CA)	16.26	0.69	0.69
	assign (segid 3A4 and resid 268 and name CA)	(segid 3A4 and resid 407 and name CB)	16.90	0.65	0.64
65	assign (segid 3A4 and resid 268 and name CA)	(segid 3A4 and resid 408 and name CA)	13.20	0.66	0.66
	assign (segid 3A4 and resid 268 and name CA)	(segid 3A4 and resid 408 and name CB)	11.83	0.69	0.68
	assign (segid 3A4 and resid 268 and name CA)	(segid 3A4 and resid 409 and name CA)	13.02	0.56	0.56
	assign (segid 3A4 and resid 268 and name CA)	(segid 3A4 and resid 409 and name CB)	12.59	0.69	0.69
	assign (segid 3A4 and resid 268 and name CA)	(segid 3A4 and resid 410 and name CA)	16.73	0.52	0.51
70	assign (segid 3A4 and resid 268 and name CA)	(segid 3A4 and resid 411 and name CA)	16.96	0.28	0.27
	assign (segid 3A4 and resid 268 and name CA)	(segid 3A4 and resid 411 and name CB)	16.99	0.38	0.37
	assign (segid 3A4 and resid 268 and name CA)	(segid 3A4 and resid 412 and name CA)	14.44	0.17	0.17
	assign (segid 3A4 and resid 268 and name CA)	(segid 3A4 and resid 413 and name CA)	12.87	1.08	1.09
	assign (segid 3A4 and resid 268 and name CA)	(segid 3A4 and resid 414 and name CA)	9.90	0.77	0.76
	assign (segid 3A4 and resid 268 and name CA)	(segid 3A4 and resid 415 and name CA)	9.07	0.93	0.93
75	assign (segid 3A4 and resid 268 and name CA)	(segid 3A4 and resid 415 and name CB)	10.02	1.46	1.45
	assign (segid 3A4 and resid 268 and name CA)	(segid 3A4 and resid 416 and name CA)	8.46	1.03	1.02
	assign (segid 3A4 and resid 268 and name CA)	(segid 3A4 and resid 417 and name CA)	11.64	0.80	0.80
	assign (segid 3A4 and resid 268 and name CA)	(segid 3A4 and resid 423 and name CA)	10.27	1.03	1.03
	assign (segid 3A4 and resid 268 and name CA)	(segid 3A4 and resid 424 and name CA)	8.83	1.16	1.16
80	assign (segid 3A4 and resid 268 and name CA)	(segid 3A4 and resid 425 and name CA)	10.04	0.93	0.94
	assign (segid 3A4 and resid 268 and name CA)	(segid 3A4 and resid 426 and name CA)	11.07	0.32	0.33
	assign (segid 3A4 and resid 268 and name CA)	(segid 3A4 and resid 427 and name CA)	13.10	1.15	1.16

	assign (segid 3A4 and resid 268 and name CA)	(segid 3A4 and resid 428 and name CA)	15.97	1.09	1.09
	assign (segid 3A4 and resid 268 and name CA)	(segid 3A4 and resid 429 and name CA)	17.50	0.82	0.82
	assign (segid 3A4 and resid 268 and name CA)	(segid 3A4 and resid 433 and name CA)	13.61	0.60	0.60
	assign (segid 3A4 and resid 268 and name CA)	(segid 3A4 and resid 434 and name CA)	10.89	0.38	0.37
5	assign (segid 3A4 and resid 268 and name CA)	(segid 3A4 and resid 435 and name CA)	8.71	0.27	0.27
	assign (segid 3A4 and resid 268 and name CA)	(segid 3A4 and resid 436 and name CA)	11.10	0.87	0.86
	assign (segid 3A4 and resid 268 and name CA)	(segid 3A4 and resid 437 and name CA)	10.36	0.56	0.56
	assign (segid 3A4 and resid 268 and name CA)	(segid 3A4 and resid 438 and name CA)	7.59	0.32	0.33
	assign (segid 3A4 and resid 268 and name CA)	(segid 3A4 and resid 439 and name CA)	9.58	0.36	0.36
10	assign (segid 3A4 and resid 268 and name CA)	(segid 3A4 and resid 440 and name CA)	9.18	0.40	0.40
	assign (segid 3A4 and resid 268 and name CB)	(segid 3A4 and resid 269 and name C)	5.44	0.05	0.05
	assign (segid 3A4 and resid 268 and name CB)	(segid 3A4 and resid 269 and name N)	4.45	0.04	0.04
	assign (segid 3A4 and resid 268 and name CB)	(segid 3A4 and resid 269 and name O)	6.29	0.04	0.04
	assign (segid 3A4 and resid 268 and name CB)	(segid 3A4 and resid 270 and name C)	6.93	0.08	0.08
15	assign (segid 3A4 and resid 268 and name CB)	(segid 3A4 and resid 270 and name CB)	6.90	0.11	0.10
	assign (segid 3A4 and resid 268 and name CB)	(segid 3A4 and resid 270 and name N)	7.48	0.14	0.14
	assign (segid 3A4 and resid 268 and name CB)	(segid 3A4 and resid 271 and name C)	5.68	0.11	0.11
	assign (segid 3A4 and resid 268 and name CB)	(segid 3A4 and resid 271 and name CA)	6.82	0.13	0.12
20	assign (segid 3A4 and resid 268 and name CB)	(segid 3A4 and resid 271 and name CB)	6.45	0.17	0.17
	assign (segid 3A4 and resid 268 and name CB)	(segid 3A4 and resid 271 and name N)	5.70	0.10	0.11
	assign (segid 3A4 and resid 268 and name CB)	(segid 3A4 and resid 272 and name CA)	5.98	0.19	0.20
	assign (segid 3A4 and resid 268 and name CB)	(segid 3A4 and resid 272 and name CB)	6.92	0.22	0.21
25	assign (segid 3A4 and resid 268 and name CB)	(segid 3A4 and resid 272 and name N)	6.25	0.16	0.16
	assign (segid 3A4 and resid 268 and name CB)	(segid 3A4 and resid 273 and name CA)	6.20	0.16	0.15
	assign (segid 3A4 and resid 268 and name CB)	(segid 3A4 and resid 273 and name CB)	9.62	0.18	0.19
	assign (segid 3A4 and resid 268 and name CB)	(segid 3A4 and resid 274 and name CA)	9.60	0.42	0.42
	assign (segid 3A4 and resid 268 and name CB)	(segid 3A4 and resid 274 and name CB)	11.86	0.55	0.54
30	assign (segid 3A4 and resid 268 and name CB)	(segid 3A4 and resid 274 and name N)	12.58	0.21	0.21
	assign (segid 3A4 and resid 268 and name CB)	(segid 3A4 and resid 275 and name CB)	14.49	0.17	0.18
	assign (segid 3A4 and resid 268 and name CB)	(segid 3A4 and resid 276 and name CA)	15.12	0.18	0.19
	assign (segid 3A4 and resid 268 and name CB)	(segid 3A4 and resid 276 and name CB)	12.80	0.18	0.18
	assign (segid 3A4 and resid 268 and name CB)	(segid 3A4 and resid 277 and name CA)	11.66	0.38	0.38
35	assign (segid 3A4 and resid 268 and name CB)	(segid 3A4 and resid 277 and name CB)	12.17	0.49	0.49
	assign (segid 3A4 and resid 268 and name CB)	(segid 3A4 and resid 278 and name CA)	11.50	0.37	0.37
	assign (segid 3A4 and resid 268 and name CB)	(segid 3A4 and resid 278 and name CB)	15.78	0.38	0.37
	assign (segid 3A4 and resid 268 and name CB)	(segid 3A4 and resid 279 and name CA)	16.44	0.32	0.31
	assign (segid 3A4 and resid 268 and name CB)	(segid 3A4 and resid 279 and name CB)	17.09	0.32	0.31
	assign (segid 3A4 and resid 268 and name CB)	(segid 3A4 and resid 280 and name CA)	16.80	0.58	0.57
40	assign (segid 3A4 and resid 268 and name CB)	(segid 3A4 and resid 280 and name CB)	15.73	0.63	0.64
	assign (segid 3A4 and resid 268 and name CB)	(segid 3A4 and resid 281 and name CA)	14.34	0.77	0.78
	assign (segid 3A4 and resid 268 and name CB)	(segid 3A4 and resid 281 and name CB)	17.19	0.74	0.74
	assign (segid 3A4 and resid 268 and name CB)	(segid 3A4 and resid 304 and name CB)	16.91	0.77	0.78
	assign (segid 3A4 and resid 268 and name CB)	(segid 3A4 and resid 305 and name CA)	18.36	0.83	0.84
45	assign (segid 3A4 and resid 268 and name CB)	(segid 3A4 and resid 305 and name CB)	16.34	0.78	0.78
	assign (segid 3A4 and resid 268 and name CB)	(segid 3A4 and resid 306 and name CA)	16.67	0.85	0.85
	assign (segid 3A4 and resid 268 and name CB)	(segid 3A4 and resid 307 and name CA)	17.74	0.97	0.96
	assign (segid 3A4 and resid 268 and name CB)	(segid 3A4 and resid 307 and name CB)	17.15	1.01	1.01
50	assign (segid 3A4 and resid 268 and name CB)	(segid 3A4 and resid 308 and name CA)	17.84	0.98	0.99
	assign (segid 3A4 and resid 268 and name CB)	(segid 3A4 and resid 308 and name CB)	13.49	1.00	0.99
	assign (segid 3A4 and resid 268 and name CB)	(segid 3A4 and resid 309 and name CA)	13.08	0.85	0.86
	assign (segid 3A4 and resid 268 and name CB)	(segid 3A4 and resid 309 and name CB)	13.26	0.88	0.88
	assign (segid 3A4 and resid 268 and name CB)	(segid 3A4 and resid 310 and name CA)	14.24	0.80	0.79
55	assign (segid 3A4 and resid 268 and name CB)	(segid 3A4 and resid 310 and name CB)	15.37	0.81	0.82
	assign (segid 3A4 and resid 268 and name CB)	(segid 3A4 and resid 311 and name CA)	16.71	0.91	0.92
	assign (segid 3A4 and resid 268 and name CB)	(segid 3A4 and resid 311 and name CB)	13.39	0.98	0.97
	assign (segid 3A4 and resid 268 and name CB)	(segid 3A4 and resid 312 and name CA)	13.38	0.80	0.80
	assign (segid 3A4 and resid 268 and name CB)	(segid 3A4 and resid 312 and name CB)	10.16	0.75	0.74
60	assign (segid 3A4 and resid 268 and name CB)	(segid 3A4 and resid 313 and name CA)	9.59	0.60	0.60
	assign (segid 3A4 and resid 268 and name CB)	(segid 3A4 and resid 313 and name CB)	12.59	0.58	0.59
	assign (segid 3A4 and resid 268 and name CB)	(segid 3A4 and resid 314 and name CA)	13.81	0.70	0.69
	assign (segid 3A4 and resid 268 and name CB)	(segid 3A4 and resid 314 and name CB)	14.16	0.79	0.79
	assign (segid 3A4 and resid 268 and name CB)	(segid 3A4 and resid 315 and name CA)	14.88	0.76	0.75
65	assign (segid 3A4 and resid 268 and name CB)	(segid 3A4 and resid 315 and name CB)	11.44	0.83	0.82
	assign (segid 3A4 and resid 268 and name CB)	(segid 3A4 and resid 316 and name CA)	10.55	0.51	0.52
	assign (segid 3A4 and resid 268 and name CB)	(segid 3A4 and resid 317 and name CA)	9.88	0.39	0.40
	assign (segid 3A4 and resid 268 and name CB)	(segid 3A4 and resid 318 and name CA)	13.12	0.24	0.25
	assign (segid 3A4 and resid 268 and name CB)	(segid 3A4 and resid 318 and name CB)	12.91	0.31	0.32
70	assign (segid 3A4 and resid 268 and name CB)	(segid 3A4 and resid 319 and name CA)	12.48	0.21	0.21
	assign (segid 3A4 and resid 268 and name CB)	(segid 3A4 and resid 319 and name CB)	16.64	0.15	0.14
	assign (segid 3A4 and resid 268 and name CB)	(segid 3A4 and resid 348 and name CA)	17.56	0.93	0.92
	assign (segid 3A4 and resid 268 and name CB)	(segid 3A4 and resid 351 and name CA)	16.95	0.67	0.67
	assign (segid 3A4 and resid 268 and name CB)	(segid 3A4 and resid 352 and name CA)	18.18	0.62	0.62
75	assign (segid 3A4 and resid 268 and name CB)	(segid 3A4 and resid 352 and name CB)	18.03	0.70	0.70
	assign (segid 3A4 and resid 268 and name CB)	(segid 3A4 and resid 360 and name CA)	17.32	0.83	0.83
	assign (segid 3A4 and resid 268 and name CB)	(segid 3A4 and resid 360 and name CB)	17.22	0.78	0.78
	assign (segid 3A4 and resid 268 and name CB)	(segid 3A4 and resid 361 and name CA)	18.06	0.94	0.94
	assign (segid 3A4 and resid 268 and name CB)	(segid 3A4 and resid 361 and name CB)	14.56	1.02	1.01
80	assign (segid 3A4 and resid 268 and name CB)	(segid 3A4 and resid 362 and name CA)	14.99	1.01	1.01
	assign (segid 3A4 and resid 268 and name CB)	(segid 3A4 and resid 362 and name CB)	13.90	1.06	1.07
	assign (segid 3A4 and resid 268 and name CB)	(segid 3A4 and resid 363 and name CA)	15.14	1.06	1.06
	assign (segid 3A4 and resid 268 and name CB)	(segid 3A4 and resid 363 and name CB)	11.61	1.03	1.03

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	assign (segid 3A4 and resid 268 and name O)	(segid 3A4 and resid 270 and name CA)	4.43	0.16	0.16
	assign (segid 3A4 and resid 268 and name O)	(segid 3A4 and resid 270 and name CB)	5.47	0.20	0.20
	assign (segid 3A4 and resid 268 and name O)	(segid 3A4 and resid 270 and name CD1)	7.54	0.19	0.19
	assign (segid 3A4 and resid 268 and name O)	(segid 3A4 and resid 270 and name CD2)	7.28	0.13	0.13
	assign (segid 3A4 and resid 268 and name O)	(segid 3A4 and resid 270 and name CG)	6.46	0.17	0.16
5	assign (segid 3A4 and resid 268 and name O)	(segid 3A4 and resid 270 and name N)	3.51	0.14	0.13
	assign (segid 3A4 and resid 268 and name O)	(segid 3A4 and resid 270 and name O)	5.04	0.17	0.17
	assign (segid 3A4 and resid 268 and name O)	(segid 3A4 and resid 271 and name C)	3.74	0.13	0.12
	assign (segid 3A4 and resid 268 and name O)	(segid 3A4 and resid 271 and name CA)	3.69	0.14	0.15
	assign (segid 3A4 and resid 268 and name O)	(segid 3A4 and resid 271 and name CB)	3.56	0.15	0.15
10	assign (segid 3A4 and resid 268 and name O)	(segid 3A4 and resid 271 and name N)	3.24	0.19	0.19
	assign (segid 3A4 and resid 268 and name O)	(segid 3A4 and resid 271 and name O)	4.88	0.13	0.13
	assign (segid 3A4 and resid 268 and name O)	(segid 3A4 and resid 272 and name C)	4.91	0.13	0.14
	assign (segid 3A4 and resid 268 and name O)	(segid 3A4 and resid 272 and name CA)	3.79	0.16	0.16
	assign (segid 3A4 and resid 268 and name O)	(segid 3A4 and resid 272 and name CB)	3.46	0.16	0.17
15	assign (segid 3A4 and resid 268 and name O)	(segid 3A4 and resid 272 and name N)	2.95	0.16	0.15
	assign (segid 3A4 and resid 268 and name O)	(segid 3A4 and resid 272 and name O)	5.96	0.13	0.12
	assign (segid 3A4 and resid 268 and name O)	(segid 3A4 and resid 273 and name C)	7.09	0.24	0.23
	assign (segid 3A4 and resid 268 and name O)	(segid 3A4 and resid 273 and name CA)	6.38	0.17	0.18
	assign (segid 3A4 and resid 268 and name O)	(segid 3A4 and resid 273 and name CB)	6.58	0.19	0.19
20	assign (segid 3A4 and resid 268 and name O)	(segid 3A4 and resid 273 and name N)	5.06	0.18	0.18
	assign (segid 3A4 and resid 268 and name O)	(segid 3A4 and resid 269 and name O)	1.23	0.01	0.01
	assign (segid 3A4 and resid 269 and name C)	(segid 3A4 and resid 270 and name C)	3.03	0.03	0.02
	assign (segid 3A4 and resid 269 and name C)	(segid 3A4 and resid 270 and name CA)	2.41	0.01	0.02
	assign (segid 3A4 and resid 269 and name C)	(segid 3A4 and resid 270 and name CB)	3.68	0.02	0.03
25	assign (segid 3A4 and resid 269 and name C)	(segid 3A4 and resid 270 and name CD1)	5.62	0.09	0.09
	assign (segid 3A4 and resid 269 and name C)	(segid 3A4 and resid 270 and name CD2)	4.70	0.09	0.09
	assign (segid 3A4 and resid 269 and name C)	(segid 3A4 and resid 270 and name CG)	4.24	0.06	0.07
	assign (segid 3A4 and resid 269 and name C)	(segid 3A4 and resid 270 and name N)	1.32	0.01	0.01
	assign (segid 3A4 and resid 269 and name C)	(segid 3A4 and resid 270 and name O)	3.91	0.07	0.08
30	assign (segid 3A4 and resid 269 and name C)	(segid 3A4 and resid 271 and name C)	4.53	0.07	0.08
	assign (segid 3A4 and resid 269 and name C)	(segid 3A4 and resid 271 and name CA)	4.45	0.05	0.06
	assign (segid 3A4 and resid 269 and name C)	(segid 3A4 and resid 271 and name CB)	5.18	0.08	0.08
	assign (segid 3A4 and resid 269 and name C)	(segid 3A4 and resid 271 and name N)	3.23	0.04	0.05
	assign (segid 3A4 and resid 269 and name C)	(segid 3A4 and resid 271 and name O)	5.65	0.11	0.11
35	assign (segid 3A4 and resid 269 and name C)	(segid 3A4 and resid 272 and name C)	4.71	0.07	0.06
	assign (segid 3A4 and resid 269 and name C)	(segid 3A4 and resid 272 and name CA)	4.46	0.13	0.13
	assign (segid 3A4 and resid 269 and name C)	(segid 3A4 and resid 272 and name CB)	4.39	0.24	0.24
	assign (segid 3A4 and resid 269 and name C)	(segid 3A4 and resid 272 and name N)	3.73	0.09	0.09
	assign (segid 3A4 and resid 269 and name C)	(segid 3A4 and resid 272 and name O)	5.80	0.07	0.06
40	assign (segid 3A4 and resid 269 and name C)	(segid 3A4 and resid 273 and name C)	5.50	0.21	0.21
	assign (segid 3A4 and resid 269 and name C)	(segid 3A4 and resid 273 and name CA)	4.96	0.12	0.12
	assign (segid 3A4 and resid 269 and name C)	(segid 3A4 and resid 273 and name CB)	4.64	0.18	0.17
	assign (segid 3A4 and resid 269 and name C)	(segid 3A4 and resid 273 and name N)	4.13	0.13	0.12
	assign (segid 3A4 and resid 269 and name C)	(segid 3A4 and resid 273 and name O)	5.48	0.23	0.23
45	assign (segid 3A4 and resid 269 and name C)	(segid 3A4 and resid 274 and name N)	6.47	0.27	0.27
	assign (segid 3A4 and resid 269 and name C)	(segid 3A4 and resid 276 and name C)	7.50	0.20	0.20
	assign (segid 3A4 and resid 269 and name C)	(segid 3A4 and resid 276 and name CA)	7.42	0.17	0.17
	assign (segid 3A4 and resid 269 and name C)	(segid 3A4 and resid 276 and name CB)	6.25	0.18	0.18
	assign (segid 3A4 and resid 269 and name C)	(segid 3A4 and resid 276 and name CG2)	6.72	0.19	0.18
50	assign (segid 3A4 and resid 269 and name C)	(segid 3A4 and resid 277 and name CB)	7.12	0.40	0.40
	assign (segid 3A4 and resid 269 and name C)	(segid 3A4 and resid 277 and name N)	6.99	0.24	0.23
	assign (segid 3A4 and resid 269 and name C)	(segid 3A4 and resid 363 and name CB)	6.56	0.83	0.84
	assign (segid 3A4 and resid 269 and name C)	(segid 3A4 and resid 363 and name CG)	5.92	0.93	0.94
	assign (segid 3A4 and resid 269 and name C)	(segid 3A4 and resid 269 and name C)	1.52	0.02	0.02
55	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 269 and name O)	2.37	0.03	0.04
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 270 and name C)	4.40	0.03	0.03
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 270 and name CA)	3.81	0.02	0.02
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 270 and name CB)	4.88	0.02	0.02
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 270 and name CD1)	6.52	0.15	0.15
60	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 270 and name CD2)	5.85	0.10	0.10
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 270 and name CG)	5.27	0.08	0.07
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 270 and name N)	2.45	0.01	0.02
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 270 and name O)	5.35	0.07	0.08
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 271 and name C)	5.43	0.09	0.08
65	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 271 and name CA)	5.39	0.06	0.06
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 271 and name CB)	5.79	0.11	0.10
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 271 and name N)	4.30	0.05	0.05
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 271 and name O)	6.57	0.11	0.12
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 272 and name C)	5.49	0.11	0.11
70	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 272 and name CA)	5.01	0.18	0.18
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 272 and name CB)	4.48	0.30	0.31
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 272 and name N)	4.46	0.12	0.11
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 272 and name O)	6.48	0.13	0.12
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 273 and name C)	6.83	0.20	0.19
75	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 273 and name CA)	6.08	0.14	0.13
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 273 and name CB)	5.62	0.19	0.20
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 273 and name N)	5.18	0.15	0.15
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 273 and name O)	6.87	0.23	0.23
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 274 and name CA)	8.80	0.34	0.34
80	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 274 and name CB)	9.84	0.40	0.40
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 275 and name CA)	10.69	0.15	0.16
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 275 and name CB)	11.20	0.15	0.15

	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 276 and name CA)	8.70	0.16	0.15
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 276 and name CB)	7.42	0.17	0.16
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 276 and name CG2)	7.71	0.14	0.15
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 277 and name CA)	8.90	0.29	0.30
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 277 and name CB)	8.60	0.41	0.40
5	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 278 and name CA)	12.48	0.24	0.24
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 278 and name CB)	13.08	0.26	0.25
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 279 and name CA)	13.30	0.28	0.27
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 279 and name CB)	12.80	0.35	0.35
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 280 and name CA)	12.38	0.45	0.46
10	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 280 and name CB)	11.11	0.51	0.52
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 281 and name CA)	14.41	0.55	0.55
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 281 and name CB)	14.26	0.51	0.50
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 282 and name CA)	17.18	0.47	0.46
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 282 and name CB)	18.24	0.67	0.66
15	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 303 and name CA)	15.07	0.71	0.71
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 304 and name CB)	14.67	0.67	0.67
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 305 and name CA)	13.42	0.67	0.66
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 305 and name CB)	14.03	0.56	0.56
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 306 and name CA)	14.99	0.71	0.71
20	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 307 and name CA)	13.79	0.89	0.89
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 307 and name CB)	14.24	0.96	0.96
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 308 and name CA)	10.14	0.86	0.87
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 308 and name CB)	9.75	0.86	0.86
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 309 and name CA)	10.96	0.67	0.66
25	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 309 and name CB)	12.19	0.68	0.68
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 310 and name CA)	12.83	0.63	0.64
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 310 and name CB)	13.99	0.69	0.68
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 311 and name CA)	10.33	0.74	0.75
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 311 and name CB)	9.92	0.85	0.86
30	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 312 and name CA)	7.95	0.48	0.47
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 312 and name CB)	7.59	0.40	0.41
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 313 and name CA)	11.27	0.35	0.35
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 313 and name CB)	12.50	0.37	0.36
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 314 and name CA)	12.24	0.44	0.44
35	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 314 and name CB)	12.55	0.57	0.56
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 315 and name CA)	9.58	0.45	0.45
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 315 and name CB)	8.31	0.53	0.53
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 316 and name CA)	9.53	0.41	0.41
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 317 and name CA)	13.03	0.26	0.25
40	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 318 and name CA)	13.96	0.32	0.31
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 318 and name CB)	13.64	0.35	0.35
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 319 and name CA)	17.66	0.32	0.31
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 319 and name CB)	18.45	0.34	0.34
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 348 and name CA)	16.60	0.66	0.66
45	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 351 and name CA)	16.49	0.44	0.44
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 352 and name CA)	16.24	0.40	0.40
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 352 and name CB)	15.79	0.49	0.49
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 357 and name CA)	18.17	0.53	0.53
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 357 and name CB)	16.90	0.49	0.50
50	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 358 and name CA)	18.66	0.74	0.74
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 359 and name CA)	16.04	0.76	0.76
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 359 and name CB)	15.74	0.83	0.82
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 360 and name CA)	14.49	0.61	0.61
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 360 and name CB)	15.58	0.56	0.56
55	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 361 and name CA)	12.17	0.68	0.69
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 361 and name CB)	12.85	0.77	0.77
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 362 and name CA)	10.58	0.82	0.83
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 362 and name CB)	11.63	0.93	0.94
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 363 and name CA)	7.80	0.95	0.95
60	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 363 and name CB)	6.31	0.96	0.95
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 363 and name CG)	5.75	1.07	1.06
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 364 and name CA)	10.26	1.03	1.03
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 364 and name CB)	11.55	1.02	1.03
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 365 and name CA)	10.90	1.02	1.02
65	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 365 and name CB)	10.50	1.01	1.00
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 381 and name CA)	18.05	0.62	0.61
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 383 and name CA)	16.95	0.41	0.42
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 397 and name CA)	18.23	0.32	0.33
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 397 and name CB)	17.97	0.31	0.32
70	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 398 and name CA)	17.12	0.33	0.33
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 398 and name CB)	17.74	0.40	0.39
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 399 and name CA)	19.01	0.28	0.29
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 400 and name CA)	17.57	0.53	0.53
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 400 and name CB)	17.80	0.63	0.62
75	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 401 and name CA)	13.96	0.44	0.44
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 402 and name CA)	14.99	0.31	0.31
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 402 and name CB)	16.07	0.28	0.28
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 403 and name CA)	17.18	0.41	0.41
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 403 and name CB)	18.40	0.44	0.44
80	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 404 and name CA)	14.88	0.65	0.66
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 404 and name CB)	14.31	0.77	0.76
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 405 and name CA)	12.12	0.54	0.54

	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 405 and name CB)	11.24	0.55	0.56
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 406 and name CA)	14.95	0.68	0.68
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 407 and name CA)	16.67	0.53	0.54
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 407 and name CB)	17.52	0.50	0.49
5	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 408 and name CA)	14.12	0.45	0.44
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 408 and name CB)	12.87	0.49	0.50
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 409 and name CA)	13.17	0.36	0.37
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 409 and name CB)	12.36	0.47	0.47
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 410 and name CA)	16.81	0.39	0.38
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 411 and name CA)	17.83	0.25	0.25
10	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 411 and name CB)	18.08	0.33	0.32
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 412 and name CA)	15.52	0.40	0.41
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 413 and name CA)	13.81	1.22	1.22
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 414 and name CA)	11.42	0.99	0.99
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 415 and name CA)	11.03	0.83	0.83
15	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 415 and name CB)	11.87	1.35	1.35
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 416 and name CA)	11.04	0.90	0.90
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 417 and name CA)	14.31	0.46	0.46
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 423 and name CA)	12.56	1.33	1.34
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 424 and name CA)	11.04	1.57	1.57
20	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 425 and name CA)	12.21	1.39	1.40
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 426 and name CA)	12.99	0.62	0.63
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 427 and name CA)	14.93	1.22	1.22
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 428 and name CA)	17.64	1.05	1.06
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 433 and name CA)	14.61	0.97	0.97
25	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 434 and name CA)	12.60	0.51	0.51
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 435 and name CA)	11.19	0.52	0.52
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 436 and name CA)	14.07	1.08	1.08
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 437 and name CA)	13.88	0.62	0.62
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 438 and name CA)	11.33	0.33	0.32
30	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 439 and name CA)	13.25	0.42	0.42
	assign (segid 3A4 and resid 269 and name CA)	(segid 3A4 and resid 440 and name CA)	12.41	0.51	0.52
	assign (segid 3A4 and resid 269 and name N)	(segid 3A4 and resid 269 and name C)	2.46	0.04	0.04
	assign (segid 3A4 and resid 269 and name N)	(segid 3A4 and resid 269 and name O)	1.45	0.02	0.02
35	assign (segid 3A4 and resid 269 and name N)	(segid 3A4 and resid 269 and name O)	3.48	0.04	0.04
	assign (segid 3A4 and resid 269 and name N)	(segid 3A4 and resid 270 and name C)	4.70	0.05	0.04
	assign (segid 3A4 and resid 269 and name N)	(segid 3A4 and resid 270 and name CA)	4.25	0.06	0.07
	assign (segid 3A4 and resid 269 and name N)	(segid 3A4 and resid 270 and name CB)	5.06	0.08	0.09
	assign (segid 3A4 and resid 269 and name N)	(segid 3A4 and resid 270 and name CD1)	6.61	0.18	0.17
40	assign (segid 3A4 and resid 269 and name N)	(segid 3A4 and resid 270 and name CD2)	6.46	0.05	0.05
	assign (segid 3A4 and resid 269 and name N)	(segid 3A4 and resid 270 and name CG)	5.57	0.10	0.09
	assign (segid 3A4 and resid 269 and name N)	(segid 3A4 and resid 270 and name N)	2.86	0.07	0.07
	assign (segid 3A4 and resid 269 and name N)	(segid 3A4 and resid 270 and name O)	5.80	0.06	0.06
	assign (segid 3A4 and resid 269 and name N)	(segid 3A4 and resid 271 and name C)	5.54	0.08	0.07
	assign (segid 3A4 and resid 269 and name N)	(segid 3A4 and resid 271 and name CA)	5.25	0.07	0.06
45	assign (segid 3A4 and resid 269 and name N)	(segid 3A4 and resid 271 and name CB)	5.27	0.12	0.11
	assign (segid 3A4 and resid 269 and name N)	(segid 3A4 and resid 271 and name N)	4.24	0.06	0.05
	assign (segid 3A4 and resid 269 and name N)	(segid 3A4 and resid 271 and name O)	6.75	0.09	0.08
	assign (segid 3A4 and resid 269 and name N)	(segid 3A4 and resid 272 and name C)	6.27	0.10	0.10
	assign (segid 3A4 and resid 269 and name N)	(segid 3A4 and resid 272 and name CA)	5.50	0.16	0.15
50	assign (segid 3A4 and resid 269 and name N)	(segid 3A4 and resid 272 and name CB)	4.99	0.25	0.24
	assign (segid 3A4 and resid 269 and name N)	(segid 3A4 and resid 272 and name N)	4.72	0.11	0.11
	assign (segid 3A4 and resid 269 and name N)	(segid 3A4 and resid 272 and name O)	7.32	0.11	0.11
	assign (segid 3A4 and resid 269 and name N)	(segid 3A4 and resid 273 and name CA)	7.15	0.13	0.13
	assign (segid 3A4 and resid 269 and name N)	(segid 3A4 and resid 273 and name CB)	6.90	0.19	0.19
55	assign (segid 3A4 and resid 269 and name N)	(segid 3A4 and resid 273 and name N)	6.09	0.14	0.15
	assign (segid 3A4 and resid 269 and name N)	(segid 3A4 and resid 270 and name C)	3.00	0.05	0.05
	assign (segid 3A4 and resid 269 and name O)	(segid 3A4 and resid 270 and name CA)	2.72	0.02	0.02
	assign (segid 3A4 and resid 269 and name O)	(segid 3A4 and resid 270 and name CB)	4.18	0.03	0.04
60	assign (segid 3A4 and resid 269 and name O)	(segid 3A4 and resid 270 and name CD1)	6.27	0.07	0.07
	assign (segid 3A4 and resid 269 and name O)	(segid 3A4 and resid 270 and name CD2)	4.97	0.10	0.10
	assign (segid 3A4 and resid 269 and name O)	(segid 3A4 and resid 270 and name CG)	4.82	0.08	0.08
	assign (segid 3A4 and resid 269 and name O)	(segid 3A4 and resid 270 and name N)	2.23	0.02	0.02
	assign (segid 3A4 and resid 269 and name O)	(segid 3A4 and resid 270 and name O)	3.54	0.13	0.12
	assign (segid 3A4 and resid 269 and name O)	(segid 3A4 and resid 271 and name C)	4.11	0.07	0.06
65	assign (segid 3A4 and resid 269 and name O)	(segid 3A4 and resid 271 and name CA)	4.41	0.04	0.05
	assign (segid 3A4 and resid 269 and name O)	(segid 3A4 and resid 271 and name CB)	5.38	0.07	0.06
	assign (segid 3A4 and resid 269 and name O)	(segid 3A4 and resid 271 and name N)	3.41	0.02	0.03
	assign (segid 3A4 and resid 269 and name O)	(segid 3A4 and resid 271 and name O)	5.10	0.09	0.09
	assign (segid 3A4 and resid 269 and name O)	(segid 3A4 and resid 272 and name C)	3.65	0.06	0.07
70	assign (segid 3A4 and resid 269 and name O)	(segid 3A4 and resid 272 and name CA)	3.70	0.10	0.10
	assign (segid 3A4 and resid 269 and name O)	(segid 3A4 and resid 272 and name CB)	3.75	0.19	0.19
	assign (segid 3A4 and resid 269 and name O)	(segid 3A4 and resid 272 and name N)	3.24	0.08	0.09
	assign (segid 3A4 and resid 269 and name O)	(segid 3A4 and resid 272 and name O)	4.70	0.07	0.07
	assign (segid 3A4 and resid 269 and name O)	(segid 3A4 and resid 273 and name C)	4.46	0.20	0.21
75	assign (segid 3A4 and resid 269 and name O)	(segid 3A4 and resid 273 and name CA)	3.78	0.12	0.12
	assign (segid 3A4 and resid 269 and name O)	(segid 3A4 and resid 273 and name CB)	3.48	0.16	0.16
	assign (segid 3A4 and resid 269 and name O)	(segid 3A4 and resid 273 and name N)	3.00	0.12	0.12
	assign (segid 3A4 and resid 269 and name O)	(segid 3A4 and resid 273 and name O)	4.57	0.21	0.24
	assign (segid 3A4 and resid 269 and name O)	(segid 3A4 and resid 274 and name C)	7.23	0.23	0.23
80	assign (segid 3A4 and resid 269 and name O)	(segid 3A4 and resid 274 and name CA)	6.52	0.32	0.32
	assign (segid 3A4 and resid 269 and name O)	(segid 3A4 and resid 274 and name N)	5.47	0.23	0.24
	assign (segid 3A4 and resid 269 and name O)	(segid 3A4 and resid 275 and name N)	7.44	0.23	0.22

	assign (segid 3A4 and resid 269 and name O) (segid 3A4 and resid 276 and name C)	7.07	0.20	0.21
	assign (segid 3A4 and resid 269 and name O) (segid 3A4 and resid 276 and name CA)	6.82	0.17	0.17
	assign (segid 3A4 and resid 269 and name O) (segid 3A4 and resid 276 and name CB)	5.68	0.18	0.18
	assign (segid 3A4 and resid 269 and name O) (segid 3A4 and resid 276 and name CG2)	6.01	0.22	0.22
5	assign (segid 3A4 and resid 269 and name O) (segid 3A4 and resid 276 and name N)	6.89	0.14	0.15
	assign (segid 3A4 and resid 269 and name O) (segid 3A4 and resid 277 and name CA)	7.21	0.30	0.31
	assign (segid 3A4 and resid 269 and name O) (segid 3A4 and resid 277 and name CB)	6.87	0.40	0.40
	assign (segid 3A4 and resid 269 and name O) (segid 3A4 and resid 277 and name N)	6.56	0.24	0.25
10	assign (segid 3A4 and resid 269 and name O) (segid 3A4 and resid 363 and name CB)	6.24	0.80	0.80
	assign (segid 3A4 and resid 269 and name O) (segid 3A4 and resid 363 and name CG)	5.79	0.88	0.88
	assign (segid 3A4 and resid 26 and name C) (segid 3A4 and resid 26 and name O)	1.24	0.00	0.00
	assign (segid 3A4 and resid 26 and name CA) (segid 3A4 and resid 26 and name C)	1.53	0.01	0.00
	assign (segid 3A4 and resid 26 and name CA) (segid 3A4 and resid 26 and name O)	2.40	0.02	0.01
15	assign (segid 3A4 and resid 26 and name CA) (segid 3A4 and resid 29 and name CA)	9.25	1.01	1.02
	assign (segid 3A4 and resid 26 and name CA) (segid 3A4 and resid 30 and name CA)	10.21	1.19	1.20
	assign (segid 3A4 and resid 26 and name CA) (segid 3A4 and resid 31 and name CA)	13.39	1.16	1.15
	assign (segid 3A4 and resid 26 and name CA) (segid 3A4 and resid 31 and name CB)	14.60	1.13	1.13
	assign (segid 3A4 and resid 26 and name CA) (segid 3A4 and resid 322 and name CA)	15.57	1.66	1.66
20	assign (segid 3A4 and resid 26 and name CA) (segid 3A4 and resid 323 and name CA)	17.18	1.55	1.56
	assign (segid 3A4 and resid 26 and name CA) (segid 3A4 and resid 324 and name CA)	16.89	1.35	1.34
	assign (segid 3A4 and resid 26 and name CA) (segid 3A4 and resid 324 and name CB)	16.68	1.39	1.39
	assign (segid 3A4 and resid 26 and name CA) (segid 3A4 and resid 32 and name CA)	14.60	1.30	1.29
	assign (segid 3A4 and resid 26 and name CA) (segid 3A4 and resid 32 and name CB)	14.06	1.31	1.31
25	assign (segid 3A4 and resid 26 and name CA) (segid 3A4 and resid 340 and name CA)	16.87	1.18	1.18
	assign (segid 3A4 and resid 26 and name CA) (segid 3A4 and resid 341 and name CA)	14.60	1.20	1.20
	assign (segid 3A4 and resid 26 and name CA) (segid 3A4 and resid 341 and name CB)	15.08	1.18	1.19
	assign (segid 3A4 and resid 26 and name CA) (segid 3A4 and resid 342 and name CA)	13.01	1.32	1.32
	assign (segid 3A4 and resid 26 and name CA) (segid 3A4 and resid 343 and name CA)	14.58	1.44	1.43
30	assign (segid 3A4 and resid 26 and name CA) (segid 3A4 and resid 343 and name CB)	16.07	1.44	1.44
	assign (segid 3A4 and resid 26 and name CA) (segid 3A4 and resid 344 and name CA)	14.31	1.65	1.65
	assign (segid 3A4 and resid 26 and name CA) (segid 3A4 and resid 344 and name CB)	13.13	1.66	1.66
	assign (segid 3A4 and resid 26 and name CA) (segid 3A4 and resid 54 and name CA)	10.97	3.48	3.47
	assign (segid 3A4 and resid 26 and name CA) (segid 3A4 and resid 54 and name CB)	11.26	3.80	3.79
35	assign (segid 3A4 and resid 26 and name CA) (segid 3A4 and resid 55 and name CA)	11.97	3.02	3.02
	assign (segid 3A4 and resid 26 and name CA) (segid 3A4 and resid 55 and name CB)	11.70	3.09	3.08
	assign (segid 3A4 and resid 26 and name CA) (segid 3A4 and resid 57 and name CA)	15.38	3.16	3.16
	assign (segid 3A4 and resid 26 and name N) (segid 3A4 and resid 26 and name C)	2.46	0.04	0.04
	assign (segid 3A4 and resid 26 and name N) (segid 3A4 and resid 26 and name CA)	1.46	0.01	0.00
40	assign (segid 3A4 and resid 26 and name N) (segid 3A4 and resid 26 and name O)	3.23	0.28	0.29
	assign (segid 3A4 and resid 270 and name C) (segid 3A4 and resid 270 and name CB)	2.49	0.05	0.04
	assign (segid 3A4 and resid 270 and name C) (segid 3A4 and resid 270 and name CD1)	4.96	0.08	0.08
	assign (segid 3A4 and resid 270 and name C) (segid 3A4 and resid 270 and name CD2)	4.31	0.04	0.04
	assign (segid 3A4 and resid 270 and name C) (segid 3A4 and resid 270 and name CG)	3.85	0.03	0.04
45	assign (segid 3A4 and resid 270 and name C) (segid 3A4 and resid 270 and name O)	1.23	0.01	0.01
	assign (segid 3A4 and resid 270 and name C) (segid 3A4 and resid 271 and name C)	3.02	0.03	0.04
	assign (segid 3A4 and resid 270 and name C) (segid 3A4 and resid 271 and name CA)	2.43	0.01	0.01
	assign (segid 3A4 and resid 270 and name C) (segid 3A4 and resid 271 and name CB)	3.69	0.04	0.03
	assign (segid 3A4 and resid 270 and name C) (segid 3A4 and resid 271 and name N)	1.33	0.01	0.01
50	assign (segid 3A4 and resid 270 and name C) (segid 3A4 and resid 271 and name O)	3.94	0.09	0.08
	assign (segid 3A4 and resid 270 and name C) (segid 3A4 and resid 272 and name C)	4.55	0.06	0.06
	assign (segid 3A4 and resid 270 and name C) (segid 3A4 and resid 272 and name CA)	4.40	0.05	0.05
	assign (segid 3A4 and resid 270 and name C) (segid 3A4 and resid 272 and name CB)	5.25	0.07	0.07
	assign (segid 3A4 and resid 270 and name C) (segid 3A4 and resid 272 and name N)	3.20	0.06	0.06
55	assign (segid 3A4 and resid 270 and name C) (segid 3A4 and resid 272 and name O)	5.73	0.05	0.06
	assign (segid 3A4 and resid 270 and name C) (segid 3A4 and resid 273 and name C)	4.37	0.19	0.19
	assign (segid 3A4 and resid 270 and name C) (segid 3A4 and resid 273 and name CA)	4.57	0.09	0.09
	assign (segid 3A4 and resid 270 and name C) (segid 3A4 and resid 273 and name CB)	5.03	0.16	0.16
	assign (segid 3A4 and resid 270 and name C) (segid 3A4 and resid 273 and name N)	3.75	0.08	0.07
60	assign (segid 3A4 and resid 270 and name C) (segid 3A4 and resid 273 and name O)	4.38	0.19	0.19
	assign (segid 3A4 and resid 270 and name C) (segid 3A4 and resid 274 and name C)	6.24	0.35	0.35
	assign (segid 3A4 and resid 270 and name C) (segid 3A4 and resid 274 and name CA)	5.34	0.46	0.47
	assign (segid 3A4 and resid 270 and name C) (segid 3A4 and resid 274 and name CB)	6.34	0.61	0.61
	assign (segid 3A4 and resid 270 and name C) (segid 3A4 and resid 274 and name N)	4.86	0.33	0.33
65	assign (segid 3A4 and resid 270 and name C) (segid 3A4 and resid 274 and name O)	6.58	0.33	0.33
	assign (segid 3A4 and resid 270 and name C) (segid 3A4 and resid 275 and name N)	6.96	0.32	0.33
	assign (segid 3A4 and resid 270 and name C) (segid 3A4 and resid 276 and name C)	6.46	0.28	0.28
	assign (segid 3A4 and resid 270 and name C) (segid 3A4 and resid 276 and name CA)	6.79	0.22	0.23
	assign (segid 3A4 and resid 270 and name C) (segid 3A4 and resid 276 and name CB)	6.17	0.20	0.21
70	assign (segid 3A4 and resid 270 and name C) (segid 3A4 and resid 276 and name CG2)	7.07	0.22	0.23
	assign (segid 3A4 and resid 270 and name C) (segid 3A4 and resid 276 and name N)	6.80	0.23	0.22
	assign (segid 3A4 and resid 270 and name C) (segid 3A4 and resid 276 and name O)	7.33	0.31	0.30
	assign (segid 3A4 and resid 270 and name C) (segid 3A4 and resid 277 and name C)	7.02	0.42	0.43
	assign (segid 3A4 and resid 270 and name C) (segid 3A4 and resid 277 and name CA)	5.60	0.42	0.41
75	assign (segid 3A4 and resid 270 and name C) (segid 3A4 and resid 277 and name CB)	4.78	0.51	0.50
	assign (segid 3A4 and resid 270 and name C) (segid 3A4 and resid 277 and name N)	5.50	0.33	0.33
	assign (segid 3A4 and resid 270 and name C) (segid 3A4 and resid 414 and name O)	7.08	0.78	0.79
	assign (segid 3A4 and resid 270 and name CA) (segid 3A4 and resid 270 and name C)	1.52	0.01	0.01
	assign (segid 3A4 and resid 270 and name CA) (segid 3A4 and resid 270 and name CB)	1.51	0.01	0.01
80	assign (segid 3A4 and resid 270 and name CA) (segid 3A4 and resid 270 and name CD1)	3.85	0.01	0.02
	assign (segid 3A4 and resid 270 and name CA) (segid 3A4 and resid 270 and name CD2)	3.05	0.02	0.02
	assign (segid 3A4 and resid 270 and name CA) (segid 3A4 and resid 270 and name CG)	2.55	0.03	0.02
	assign (segid 3A4 and resid 270 and name CA) (segid 3A4 and resid 270 and name O)	2.37	0.03	0.03
	assign (segid 3A4 and resid 270 and name CA) (segid 3A4 and resid 271 and name C)	4.40	0.03	0.02

	assign (segid 3A4 and resid 270 and name CA)	(segid 3A4 and resid 271 and name CA)	3.82	0.02	0.02
	assign (segid 3A4 and resid 270 and name CA)	(segid 3A4 and resid 271 and name CB)	4.86	0.07	0.06
	assign (segid 3A4 and resid 270 and name CA)	(segid 3A4 and resid 271 and name N)	2.45	0.03	0.03
	assign (segid 3A4 and resid 270 and name CA)	(segid 3A4 and resid 271 and name O)	5.37	0.08	0.09
5	assign (segid 3A4 and resid 270 and name CA)	(segid 3A4 and resid 272 and name C)	5.37	0.05	0.04
	assign (segid 3A4 and resid 270 and name CA)	(segid 3A4 and resid 272 and name CA)	5.34	0.05	0.05
	assign (segid 3A4 and resid 270 and name CA)	(segid 3A4 and resid 272 and name CB)	5.89	0.15	0.15
	assign (segid 3A4 and resid 270 and name CA)	(segid 3A4 and resid 272 and name N)	4.26	0.04	0.05
	assign (segid 3A4 and resid 270 and name CA)	(segid 3A4 and resid 272 and name O)	6.52	0.05	0.06
10	assign (segid 3A4 and resid 270 and name CA)	(segid 3A4 and resid 273 and name C)	4.86	0.19	0.19
	assign (segid 3A4 and resid 270 and name CA)	(segid 3A4 and resid 273 and name CA)	5.02	0.10	0.09
	assign (segid 3A4 and resid 270 and name CA)	(segid 3A4 and resid 273 and name CB)	5.03	0.18	0.17
	assign (segid 3A4 and resid 270 and name CA)	(segid 3A4 and resid 273 and name N)	4.42	0.07	0.06
	assign (segid 3A4 and resid 270 and name CA)	(segid 3A4 and resid 273 and name O)	4.55	0.20	0.20
15	assign (segid 3A4 and resid 270 and name CA)	(segid 3A4 and resid 274 and name C)	6.74	0.34	0.33
	assign (segid 3A4 and resid 270 and name CA)	(segid 3A4 and resid 274 and name CA)	6.12	0.46	0.46
	assign (segid 3A4 and resid 270 and name CA)	(segid 3A4 and resid 274 and name CB)	7.32	0.57	0.57
	assign (segid 3A4 and resid 270 and name CA)	(segid 3A4 and resid 274 and name N)	5.65	0.32	0.31
	assign (segid 3A4 and resid 270 and name CA)	(segid 3A4 and resid 274 and name O)	6.98	0.29	0.30
20	assign (segid 3A4 and resid 270 and name CA)	(segid 3A4 and resid 275 and name CA)	8.24	0.25	0.25
	assign (segid 3A4 and resid 270 and name CA)	(segid 3A4 and resid 275 and name CB)	9.16	0.23	0.24
	assign (segid 3A4 and resid 270 and name CA)	(segid 3A4 and resid 275 and name N)	7.34	0.32	0.31
	assign (segid 3A4 and resid 270 and name CA)	(segid 3A4 and resid 276 and name C)	5.92	0.24	0.25
	assign (segid 3A4 and resid 270 and name CA)	(segid 3A4 and resid 276 and name CA)	6.27	0.21	0.21
25	assign (segid 3A4 and resid 270 and name CA)	(segid 3A4 and resid 276 and name CB)	5.46	0.20	0.20
	assign (segid 3A4 and resid 270 and name CA)	(segid 3A4 and resid 276 and name CG2)	6.41	0.21	0.20
	assign (segid 3A4 and resid 270 and name CA)	(segid 3A4 and resid 276 and name N)	6.58	0.20	0.20
	assign (segid 3A4 and resid 270 and name CA)	(segid 3A4 and resid 276 and name O)	6.66	0.26	0.27
	assign (segid 3A4 and resid 270 and name CA)	(segid 3A4 and resid 277 and name C)	6.83	0.33	0.33
30	assign (segid 3A4 and resid 270 and name CA)	(segid 3A4 and resid 277 and name CA)	5.34	0.33	0.33
	assign (segid 3A4 and resid 270 and name CA)	(segid 3A4 and resid 277 and name CB)	4.88	0.40	0.41
	assign (segid 3A4 and resid 270 and name CA)	(segid 3A4 and resid 277 and name N)	5.18	0.27	0.27
	assign (segid 3A4 and resid 270 and name CA)	(segid 3A4 and resid 278 and name CA)	8.98	0.31	0.31
	assign (segid 3A4 and resid 270 and name CA)	(segid 3A4 and resid 278 and name CB)	9.71	0.33	0.32
35	assign (segid 3A4 and resid 270 and name CA)	(segid 3A4 and resid 279 and name CA)	10.27	0.33	0.33
	assign (segid 3A4 and resid 270 and name CA)	(segid 3A4 and resid 279 and name CB)	10.09	0.35	0.35
	assign (segid 3A4 and resid 270 and name CA)	(segid 3A4 and resid 280 and name CA)	9.32	0.51	0.50
	assign (segid 3A4 and resid 270 and name CA)	(segid 3A4 and resid 280 and name CB)	8.10	0.56	0.57
40	assign (segid 3A4 and resid 270 and name CA)	(segid 3A4 and resid 281 and name CA)	10.85	0.60	0.60
	assign (segid 3A4 and resid 270 and name CA)	(segid 3A4 and resid 281 and name CB)	10.57	0.54	0.55
	assign (segid 3A4 and resid 270 and name CA)	(segid 3A4 and resid 282 and name CA)	13.74	0.54	0.55
	assign (segid 3A4 and resid 270 and name CA)	(segid 3A4 and resid 303 and name CA)	16.18	0.63	0.62
	assign (segid 3A4 and resid 270 and name CA)	(segid 3A4 and resid 303 and name CB)	17.30	0.65	0.64
45	assign (segid 3A4 and resid 270 and name CA)	(segid 3A4 and resid 304 and name CA)	13.16	0.68	0.69
	assign (segid 3A4 and resid 270 and name CA)	(segid 3A4 and resid 304 and name CB)	12.58	0.70	0.69
	assign (segid 3A4 and resid 270 and name CA)	(segid 3A4 and resid 305 and name CA)	11.59	0.63	0.64
	assign (segid 3A4 and resid 270 and name CA)	(segid 3A4 and resid 305 and name CB)	12.03	0.56	0.57
	assign (segid 3A4 and resid 270 and name CA)	(segid 3A4 and resid 306 and name CA)	14.02	0.62	0.61
	assign (segid 3A4 and resid 270 and name CA)	(segid 3A4 and resid 307 and name CA)	13.19	0.77	0.77
50	assign (segid 3A4 and resid 270 and name CA)	(segid 3A4 and resid 307 and name CB)	13.46	0.85	0.84
	assign (segid 3A4 and resid 270 and name CA)	(segid 3A4 and resid 308 and name CA)	9.50	0.74	0.74
	assign (segid 3A4 and resid 270 and name CA)	(segid 3A4 and resid 308 and name CB)	8.60	0.78	0.77
	assign (segid 3A4 and resid 270 and name CA)	(segid 3A4 and resid 309 and name CA)	10.98	0.53	0.54
	assign (segid 3A4 and resid 270 and name CA)	(segid 3A4 and resid 309 and name CB)	12.02	0.57	0.58
55	assign (segid 3A4 and resid 270 and name CA)	(segid 3A4 and resid 310 and name CA)	13.52	0.46	0.47
	assign (segid 3A4 and resid 270 and name CA)	(segid 3A4 and resid 310 and name CB)	14.51	0.54	0.53
	assign (segid 3A4 and resid 270 and name CA)	(segid 3A4 and resid 311 and name CA)	11.47	0.51	0.51
	assign (segid 3A4 and resid 270 and name CA)	(segid 3A4 and resid 311 and name CB)	10.77	0.62	0.62
	assign (segid 3A4 and resid 270 and name CA)	(segid 3A4 and resid 312 and name CA)	9.62	0.27	0.27
60	assign (segid 3A4 and resid 270 and name CA)	(segid 3A4 and resid 312 and name CB)	8.93	0.27	0.27
	assign (segid 3A4 and resid 270 and name CA)	(segid 3A4 and resid 313 and name CA)	13.22	0.23	0.23
	assign (segid 3A4 and resid 270 and name CA)	(segid 3A4 and resid 313 and name CB)	14.18	0.23	0.24
	assign (segid 3A4 and resid 270 and name CA)	(segid 3A4 and resid 314 and name CA)	14.51	0.28	0.28
	assign (segid 3A4 and resid 270 and name CA)	(segid 3A4 and resid 314 and name CB)	14.62	0.38	0.37
65	assign (segid 3A4 and resid 270 and name CA)	(segid 3A4 and resid 315 and name CA)	12.43	0.38	0.38
	assign (segid 3A4 and resid 270 and name CA)	(segid 3A4 and resid 315 and name CB)	11.08	0.44	0.45
	assign (segid 3A4 and resid 270 and name CA)	(segid 3A4 and resid 316 and name CA)	12.69	0.49	0.48
	assign (segid 3A4 and resid 270 and name CA)	(segid 3A4 and resid 317 and name CA)	15.98	0.33	0.33
	assign (segid 3A4 and resid 270 and name CA)	(segid 3A4 and resid 318 and name CA)	16.86	0.25	0.25
70	assign (segid 3A4 and resid 270 and name CA)	(segid 3A4 and resid 318 and name CB)	16.34	0.30	0.29
	assign (segid 3A4 and resid 270 and name CA)	(segid 3A4 and resid 351 and name CA)	19.18	0.31	0.32
	assign (segid 3A4 and resid 270 and name CA)	(segid 3A4 and resid 352 and name CA)	19.15	0.36	0.37
	assign (segid 3A4 and resid 270 and name CA)	(segid 3A4 and resid 352 and name CB)	18.90	0.47	0.46
	assign (segid 3A4 and resid 270 and name CA)	(segid 3A4 and resid 357 and name CB)	18.94	0.35	0.35
75	assign (segid 3A4 and resid 270 and name CA)	(segid 3A4 and resid 359 and name CA)	18.02	0.61	0.61
	assign (segid 3A4 and resid 270 and name CA)	(segid 3A4 and resid 359 and name CB)	17.48	0.67	0.66
	assign (segid 3A4 and resid 270 and name CA)	(segid 3A4 and resid 360 and name CA)	16.95	0.47	0.46
	assign (segid 3A4 and resid 270 and name CA)	(segid 3A4 and resid 360 and name CB)	18.18	0.45	0.45
	assign (segid 3A4 and resid 270 and name CA)	(segid 3A4 and resid 361 and name CA)	14.96	0.57	0.58
80	assign (segid 3A4 and resid 270 and name CA)	(segid 3A4 and resid 361 and name CB)	15.75	0.67	0.67
	assign (segid 3A4 and resid 270 and name CA)	(segid 3A4 and resid 362 and name CA)	12.64	0.65	0.64
	assign (segid 3A4 and resid 270 and name CA)	(segid 3A4 and resid 362 and name CB)	13.37	0.77	0.78
	assign (segid 3A4 and resid 270 and name CA)	(segid 3A4 and resid 363 and name CA)	9.49	0.67	0.67

	assign (segid 3A4 and resid 270 and name CA) (segid 3A4 and resid 363 and name CB)	8.13	0.65	0.64
	assign (segid 3A4 and resid 270 and name CA) (segid 3A4 and resid 364 and name CA)	10.73	0.89	0.88
	assign (segid 3A4 and resid 270 and name CA) (segid 3A4 and resid 364 and name CB)	12.11	0.89	0.89
	assign (segid 3A4 and resid 270 and name CA) (segid 3A4 and resid 365 and name CA)	10.54	0.95	0.95
	assign (segid 3A4 and resid 270 and name CA) (segid 3A4 and resid 365 and name CB)	9.66	0.99	0.99
5	assign (segid 3A4 and resid 270 and name CA) (segid 3A4 and resid 383 and name CA)	19.21	0.29	0.29
	assign (segid 3A4 and resid 270 and name CA) (segid 3A4 and resid 397 and name CA)	18.75	0.39	0.38
	assign (segid 3A4 and resid 270 and name CA) (segid 3A4 and resid 397 and name CB)	18.78	0.37	0.37
	assign (segid 3A4 and resid 270 and name CA) (segid 3A4 and resid 398 and name CA)	17.20	0.41	0.40
	assign (segid 3A4 and resid 270 and name CA) (segid 3A4 and resid 398 and name CB)	17.83	0.46	0.46
10	assign (segid 3A4 and resid 270 and name CA) (segid 3A4 and resid 399 and name CA)	18.46	0.38	0.37
	assign (segid 3A4 and resid 270 and name CA) (segid 3A4 and resid 400 and name CA)	17.11	0.57	0.57
	assign (segid 3A4 and resid 270 and name CA) (segid 3A4 and resid 400 and name CB)	17.60	0.64	0.64
	assign (segid 3A4 and resid 270 and name CA) (segid 3A4 and resid 401 and name CA)	13.56	0.48	0.49
	assign (segid 3A4 and resid 270 and name CA) (segid 3A4 and resid 402 and name CA)	13.81	0.43	0.43
15	assign (segid 3A4 and resid 270 and name CA) (segid 3A4 and resid 402 and name CB)	14.92	0.41	0.41
	assign (segid 3A4 and resid 270 and name CA) (segid 3A4 and resid 403 and name CA)	15.62	0.52	0.52
	assign (segid 3A4 and resid 270 and name CA) (segid 3A4 and resid 403 and name CB)	16.97	0.54	0.54
	assign (segid 3A4 and resid 270 and name CA) (segid 3A4 and resid 404 and name CA)	13.42	0.74	0.74
	assign (segid 3A4 and resid 270 and name CA) (segid 3A4 and resid 404 and name CB)	13.20	0.84	0.84
20	assign (segid 3A4 and resid 270 and name CA) (segid 3A4 and resid 405 and name CA)	10.23	0.59	0.58
	assign (segid 3A4 and resid 270 and name CA) (segid 3A4 and resid 405 and name CB)	9.53	0.54	0.54
	assign (segid 3A4 and resid 270 and name CA) (segid 3A4 and resid 406 and name CA)	12.45	0.72	0.73
	assign (segid 3A4 and resid 270 and name CA) (segid 3A4 and resid 407 and name CA)	14.11	0.57	0.58
	assign (segid 3A4 and resid 270 and name CA) (segid 3A4 and resid 407 and name CB)	15.16	0.53	0.52
25	assign (segid 3A4 and resid 270 and name CA) (segid 3A4 and resid 408 and name CA)	11.56	0.47	0.47
	assign (segid 3A4 and resid 270 and name CA) (segid 3A4 and resid 408 and name CB)	10.55	0.54	0.53
	assign (segid 3A4 and resid 270 and name CA) (segid 3A4 and resid 409 and name CA)	9.95	0.35	0.35
	assign (segid 3A4 and resid 270 and name CA) (segid 3A4 and resid 409 and name CB)	9.08	0.45	0.45
30	assign (segid 3A4 and resid 270 and name CA) (segid 3A4 and resid 409 and name CD2)	7.00	0.44	0.43
	assign (segid 3A4 and resid 270 and name CA) (segid 3A4 and resid 410 and name CA)	13.45	0.36	0.37
	assign (segid 3A4 and resid 270 and name CA) (segid 3A4 and resid 411 and name CA)	14.67	0.34	0.33
	assign (segid 3A4 and resid 270 and name CA) (segid 3A4 and resid 411 and name CB)	15.11	0.32	0.33
	assign (segid 3A4 and resid 270 and name CA) (segid 3A4 and resid 412 and name CA)	12.35	0.58	0.59
	assign (segid 3A4 and resid 270 and name CA) (segid 3A4 and resid 413 and name CA)	10.67	1.19	1.20
35	assign (segid 3A4 and resid 270 and name CA) (segid 3A4 and resid 414 and name CA)	8.97	0.91	0.91
	assign (segid 3A4 and resid 270 and name CA) (segid 3A4 and resid 415 and name CA)	9.46	0.58	0.58
	assign (segid 3A4 and resid 270 and name CA) (segid 3A4 and resid 415 and name CB)	10.35	0.78	0.79
	assign (segid 3A4 and resid 270 and name CA) (segid 3A4 and resid 416 and name CA)	10.54	1.03	1.03
	assign (segid 3A4 and resid 270 and name CA) (segid 3A4 and resid 417 and name CA)	14.02	0.64	0.63
40	assign (segid 3A4 and resid 270 and name CA) (segid 3A4 and resid 423 and name CA)	14.51	1.21	1.22
	assign (segid 3A4 and resid 270 and name CA) (segid 3A4 and resid 424 and name CA)	13.54	1.29	1.29
	assign (segid 3A4 and resid 270 and name CA) (segid 3A4 and resid 425 and name CA)	15.08	1.20	1.21
	assign (segid 3A4 and resid 270 and name CA) (segid 3A4 and resid 426 and name CA)	16.20	0.45	0.46
	assign (segid 3A4 and resid 270 and name CA) (segid 3A4 and resid 433 and name CA)	17.82	0.81	0.81
45	assign (segid 3A4 and resid 270 and name CA) (segid 3A4 and resid 434 and name CA)	15.57	0.42	0.41
	assign (segid 3A4 and resid 270 and name CA) (segid 3A4 and resid 435 and name CA)	13.94	0.36	0.36
	assign (segid 3A4 and resid 270 and name CA) (segid 3A4 and resid 436 and name CA)	16.46	0.88	0.88
	assign (segid 3A4 and resid 270 and name CA) (segid 3A4 and resid 437 and name CA)	15.63	0.53	0.54
	assign (segid 3A4 and resid 270 and name CA) (segid 3A4 and resid 438 and name CA)	12.52	0.37	0.37
50	assign (segid 3A4 and resid 270 and name CA) (segid 3A4 and resid 439 and name CA)	13.56	0.45	0.46
	assign (segid 3A4 and resid 270 and name CA) (segid 3A4 and resid 440 and name CA)	11.69	0.55	0.55
	assign (segid 3A4 and resid 270 and name CB) (segid 3A4 and resid 270 and name CD1)	2.49	0.03	0.02
	assign (segid 3A4 and resid 270 and name CB) (segid 3A4 and resid 270 and name CD2)	2.49	0.03	0.02
	assign (segid 3A4 and resid 270 and name CB) (segid 3A4 and resid 270 and name CG)	1.52	0.01	0.01
55	assign (segid 3A4 and resid 270 and name CB) (segid 3A4 and resid 271 and name C)	5.44	0.06	0.06
	assign (segid 3A4 and resid 270 and name CB) (segid 3A4 and resid 271 and name CA)	4.54	0.09	0.08
	assign (segid 3A4 and resid 270 and name CB) (segid 3A4 and resid 271 and name CB)	5.40	0.15	0.15
	assign (segid 3A4 and resid 270 and name CB) (segid 3A4 and resid 271 and name N)	3.24	0.07	0.06
	assign (segid 3A4 and resid 270 and name CB) (segid 3A4 and resid 271 and name O)	6.37	0.10	0.11
60	assign (segid 3A4 and resid 270 and name CB) (segid 3A4 and resid 272 and name C)	6.79	0.08	0.07
	assign (segid 3A4 and resid 270 and name CB) (segid 3A4 and resid 272 and name CA)	6.72	0.03	0.03
	assign (segid 3A4 and resid 270 and name CB) (segid 3A4 and resid 272 and name CB)	7.31	0.14	0.14
	assign (segid 3A4 and resid 270 and name CB) (segid 3A4 and resid 272 and name N)	5.53	0.03	0.04
	assign (segid 3A4 and resid 270 and name CB) (segid 3A4 and resid 273 and name C)	5.90	0.16	0.17
65	assign (segid 3A4 and resid 270 and name CB) (segid 3A4 and resid 273 and name CA)	6.31	0.10	0.10
	assign (segid 3A4 and resid 270 and name CB) (segid 3A4 and resid 273 and name CB)	6.32	0.18	0.19
	assign (segid 3A4 and resid 270 and name CB) (segid 3A4 and resid 273 and name N)	5.81	0.08	0.08
	assign (segid 3A4 and resid 270 and name CB) (segid 3A4 and resid 273 and name O)	5.41	0.16	0.15
70	assign (segid 3A4 and resid 270 and name CB) (segid 3A4 and resid 274 and name C)	7.24	0.36	0.36
	assign (segid 3A4 and resid 270 and name CB) (segid 3A4 and resid 274 and name CA)	6.76	0.48	0.49
	assign (segid 3A4 and resid 270 and name CB) (segid 3A4 and resid 274 and name CB)	7.97	0.64	0.64
	assign (segid 3A4 and resid 270 and name CB) (segid 3A4 and resid 274 and name N)	6.58	0.32	0.31
	assign (segid 3A4 and resid 270 and name CB) (segid 3A4 and resid 274 and name O)	7.24	0.32	0.32
75	assign (segid 3A4 and resid 270 and name CB) (segid 3A4 and resid 275 and name CA)	8.76	0.26	0.26
	assign (segid 3A4 and resid 270 and name CB) (segid 3A4 and resid 275 and name CB)	9.83	0.24	0.25
	assign (segid 3A4 and resid 270 and name CB) (segid 3A4 and resid 276 and name C)	5.86	0.20	0.21
	assign (segid 3A4 and resid 270 and name CB) (segid 3A4 and resid 276 and name CA)	6.53	0.18	0.19
	assign (segid 3A4 and resid 270 and name CB) (segid 3A4 and resid 276 and name CB)	5.90	0.18	0.17
80	assign (segid 3A4 and resid 270 and name CB) (segid 3A4 and resid 276 and name CG2)	7.07	0.17	0.17
	assign (segid 3A4 and resid 270 and name CB) (segid 3A4 and resid 276 and name N)	7.03	0.20	0.20
	assign (segid 3A4 and resid 270 and name CB) (segid 3A4 and resid 276 and name O)	6.38	0.23	0.22
	assign (segid 3A4 and resid 270 and name CB) (segid 3A4 and resid 277 and name C)	6.31	0.32	0.32

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	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 277 and name CA)	4.89	0.30	0.30
	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 277 and name CB)	4.48	0.38	0.38
	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 277 and name N)	5.10	0.25	0.25
	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 277 and name O)	6.76	0.37	0.38
5	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 278 and name CA)	8.67	0.32	0.31
	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 278 and name CB)	9.53	0.34	0.34
	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 279 and name CA)	9.90	0.33	0.32
	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 279 and name CB)	9.87	0.33	0.34
	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 280 and name CA)	8.47	0.52	0.51
10	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 280 and name CB)	7.16	0.56	0.57
	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 281 and name CA)	9.83	0.63	0.64
	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 281 and name CB)	9.61	0.57	0.58
	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 282 and name CA)	12.94	0.58	0.58
	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 303 and name CA)	15.31	0.68	0.67
15	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 303 and name CB)	16.48	0.67	0.68
	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 304 and name CA)	12.48	0.68	0.67
	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 304 and name CB)	11.96	0.71	0.70
	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 305 and name CA)	10.64	0.63	0.63
20	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 305 and name CB)	10.94	0.58	0.58
	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 306 and name CA)	13.22	0.57	0.58
	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 307 and name CA)	12.77	0.68	0.68
	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 307 and name CB)	13.09	0.74	0.75
	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 308 and name CA)	9.09	0.66	0.66
	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 308 and name CB)	8.02	0.71	0.72
25	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 309 and name CA)	10.40	0.47	0.48
	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 309 and name CB)	11.30	0.53	0.54
	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 310 and name CA)	13.25	0.38	0.39
	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 310 and name CB)	14.24	0.44	0.45
30	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 311 and name CA)	11.59	0.41	0.42
	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 311 and name CB)	10.95	0.51	0.52
	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 312 and name CA)	9.69	0.24	0.24
	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 312 and name CB)	8.81	0.29	0.28
	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 313 and name CA)	13.20	0.25	0.25
35	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 313 and name CB)	14.04	0.26	0.25
	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 314 and name CA)	14.81	0.25	0.25
	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 314 and name CB)	14.95	0.30	0.29
	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 315 and name CA)	13.04	0.41	0.40
	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 315 and name CB)	11.75	0.46	0.46
40	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 316 and name CA)	13.15	0.55	0.56
	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 317 and name CA)	16.27	0.42	0.42
	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 318 and name CA)	17.00	0.24	0.24
	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 318 and name CB)	16.37	0.30	0.30
	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 359 and name CA)	19.06	0.53	0.52
	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 359 and name CB)	18.53	0.59	0.59
45	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 360 and name CA)	17.89	0.43	0.43
	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 360 and name CB)	19.11	0.43	0.44
	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 361 and name CA)	16.09	0.58	0.59
	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 361 and name CB)	16.95	0.69	0.68
	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 362 and name CA)	13.78	0.60	0.59
50	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 362 and name CB)	14.50	0.71	0.70
	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 363 and name CA)	10.45	0.59	0.58
	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 363 and name CB)	9.13	0.56	0.56
	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 364 and name CA)	11.39	0.77	0.78
	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 364 and name CB)	12.83	0.78	0.77
55	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 365 and name CA)	10.71	0.90	0.89
	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 365 and name CB)	9.68	0.96	0.97
	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 383 and name CA)	19.22	0.26	0.26
	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 397 and name CA)	17.92	0.45	0.44
	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 397 and name CB)	18.05	0.42	0.42
60	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 398 and name CA)	16.32	0.46	0.47
	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 398 and name CB)	17.00	0.50	0.51
	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 399 and name CA)	17.35	0.46	0.45
	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 399 and name CB)	18.79	0.45	0.46
	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 400 and name CA)	15.97	0.62	0.61
65	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 400 and name CB)	16.51	0.68	0.68
	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 401 and name CA)	12.50	0.54	0.54
	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 402 and name CA)	12.61	0.51	0.51
	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 402 and name CB)	13.76	0.49	0.49
	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 403 and name CA)	14.26	0.58	0.57
70	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 403 and name CB)	15.61	0.59	0.59
	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 404 and name CA)	12.05	0.76	0.77
	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 404 and name CB)	11.91	0.86	0.85
	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 405 and name CA)	8.82	0.62	0.62
	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 405 and name CB)	8.21	0.57	0.57
75	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 406 and name CA)	11.01	0.75	0.76
	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 407 and name CA)	12.62	0.58	0.59
	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 407 and name CB)	13.67	0.52	0.53
	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 408 and name CA)	10.12	0.43	0.43
80	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 408 and name CB)	9.13	0.49	0.50
	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 409 and name CA)	8.55	0.31	0.31
	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 409 and name CB)	7.69	0.45	0.45
	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 409 and name CD2)	5.67	0.38	0.38
	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 409 and name CG)	6.38	0.51	0.50

	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 410 and name CA)	12.08	0.35	0.35
	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 411 and name CA)	13.34	0.29	0.29
	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 411 and name CB)	13.76	0.30	0.29
	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 412 and name CA)	11.21	0.56	0.57
5	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 413 and name CA)	10.05	1.09	1.09
	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 414 and name CA)	8.53	0.87	0.87
	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 415 and name CA)	9.52	0.64	0.63
	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 415 and name CB)	10.48	0.68	0.68
	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 416 and name CA)	10.88	1.17	1.16
	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 417 and name CA)	14.39	0.83	0.83
10	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 423 and name CA)	15.40	1.22	1.21
	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 424 and name CA)	14.38	1.27	1.28
	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 425 and name CA)	15.83	1.07	1.07
	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 426 and name CA)	16.88	0.41	0.41
	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 433 and name CA)	18.14	0.73	0.74
15	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 434 and name CA)	15.81	0.41	0.40
	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 435 and name CA)	14.24	0.29	0.29
	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 436 and name CA)	16.69	0.73	0.73
	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 437 and name CA)	15.79	0.47	0.46
	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 438 and name CA)	12.65	0.33	0.34
20	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 439 and name CA)	13.58	0.40	0.40
	assign (segid 3A4 and resid 270 and name CB)	(segid 3A4 and resid 440 and name CA)	11.51	0.46	0.46
	assign (segid 3A4 and resid 270 and name CD1)	(segid 3A4 and resid 270 and name CD2)	2.47	0.06	0.06
	assign (segid 3A4 and resid 270 and name CD1)	(segid 3A4 and resid 271 and name CA)	6.87	0.15	0.16
	assign (segid 3A4 and resid 270 and name CD1)	(segid 3A4 and resid 271 and name CB)	7.55	0.22	0.22
25	assign (segid 3A4 and resid 270 and name CD1)	(segid 3A4 and resid 271 and name N)	5.62	0.10	0.10
	assign (segid 3A4 and resid 270 and name CD1)	(segid 3A4 and resid 273 and name O)	7.12	0.16	0.15
	assign (segid 3A4 and resid 270 and name CD1)	(segid 3A4 and resid 276 and name C)	6.16	0.24	0.24
	assign (segid 3A4 and resid 270 and name CD1)	(segid 3A4 and resid 276 and name CA)	7.10	0.21	0.22
	assign (segid 3A4 and resid 270 and name CD1)	(segid 3A4 and resid 276 and name CB)	6.59	0.22	0.22
30	assign (segid 3A4 and resid 270 and name CD1)	(segid 3A4 and resid 276 and name O)	6.20	0.24	0.25
	assign (segid 3A4 and resid 270 and name CD1)	(segid 3A4 and resid 277 and name C)	6.33	0.29	0.30
	assign (segid 3A4 and resid 270 and name CD1)	(segid 3A4 and resid 277 and name CA)	5.19	0.31	0.30
	assign (segid 3A4 and resid 270 and name CD1)	(segid 3A4 and resid 277 and name CB)	5.24	0.36	0.36
	assign (segid 3A4 and resid 270 and name CD1)	(segid 3A4 and resid 277 and name N)	5.70	0.30	0.29
35	assign (segid 3A4 and resid 270 and name CD1)	(segid 3A4 and resid 277 and name O)	6.37	0.33	0.32
	assign (segid 3A4 and resid 270 and name CD1)	(segid 3A4 and resid 280 and name CB)	5.73	0.54	0.54
	assign (segid 3A4 and resid 270 and name CD1)	(segid 3A4 and resid 308 and name CB)	6.46	0.61	0.62
	assign (segid 3A4 and resid 270 and name CD1)	(segid 3A4 and resid 405 and name CA)	6.54	0.56	0.57
	assign (segid 3A4 and resid 270 and name CD1)	(segid 3A4 and resid 405 and name CB)	5.84	0.57	0.57
40	assign (segid 3A4 and resid 270 and name CD1)	(segid 3A4 and resid 405 and name O)	6.53	0.54	0.53
	assign (segid 3A4 and resid 270 and name CD1)	(segid 3A4 and resid 409 and name CA)	7.20	0.29	0.30
	assign (segid 3A4 and resid 270 and name CD1)	(segid 3A4 and resid 409 and name CB)	6.24	0.28	0.28
	assign (segid 3A4 and resid 270 and name CD1)	(segid 3A4 and resid 409 and name CD2)	4.71	0.55	0.56
	assign (segid 3A4 and resid 270 and name CD1)	(segid 3A4 and resid 409 and name CG)	4.93	0.30	0.30
45	assign (segid 3A4 and resid 270 and name CD1)	(segid 3A4 and resid 409 and name N)	7.37	0.10	0.10
	assign (segid 3A4 and resid 270 and name CD1)	(segid 3A4 and resid 271 and name C)	7.27	0.03	0.04
	assign (segid 3A4 and resid 270 and name CD2)	(segid 3A4 and resid 271 and name CA)	6.67	0.05	0.06
	assign (segid 3A4 and resid 270 and name CD2)	(segid 3A4 and resid 271 and name CB)	7.72	0.12	0.12
	assign (segid 3A4 and resid 270 and name CD2)	(segid 3A4 and resid 271 and name N)	5.39	0.03	0.03
50	assign (segid 3A4 and resid 270 and name CD2)	(segid 3A4 and resid 272 and name C)	7.74	0.16	0.17
	assign (segid 3A4 and resid 270 and name CD2)	(segid 3A4 and resid 272 and name N)	7.18	0.11	0.11
	assign (segid 3A4 and resid 270 and name CD2)	(segid 3A4 and resid 273 and name C)	6.00	0.16	0.17
	assign (segid 3A4 and resid 270 and name CD2)	(segid 3A4 and resid 273 and name CA)	6.53	0.16	0.17
	assign (segid 3A4 and resid 270 and name CD2)	(segid 3A4 and resid 273 and name CB)	6.11	0.24	0.24
55	assign (segid 3A4 and resid 270 and name CD2)	(segid 3A4 and resid 273 and name N)	6.55	0.15	0.14
	assign (segid 3A4 and resid 270 and name CD2)	(segid 3A4 and resid 273 and name O)	5.10	0.18	0.17
	assign (segid 3A4 and resid 270 and name CD2)	(segid 3A4 and resid 274 and name C)	6.99	0.32	0.31
	assign (segid 3A4 and resid 270 and name CD2)	(segid 3A4 and resid 274 and name CA)	7.02	0.43	0.42
	assign (segid 3A4 and resid 270 and name CD2)	(segid 3A4 and resid 274 and name N)	6.91	0.26	0.26
60	assign (segid 3A4 and resid 270 and name CD2)	(segid 3A4 and resid 274 and name O)	6.85	0.27	0.27
	assign (segid 3A4 and resid 270 and name CD2)	(segid 3A4 and resid 275 and name C)	6.83	0.17	0.18
	assign (segid 3A4 and resid 270 and name CD2)	(segid 3A4 and resid 275 and name N)	7.47	0.29	0.28
	assign (segid 3A4 and resid 270 and name CD2)	(segid 3A4 and resid 275 and name O)	7.20	0.17	0.17
	assign (segid 3A4 and resid 270 and name CD2)	(segid 3A4 and resid 276 and name C)	4.17	0.16	0.15
65	assign (segid 3A4 and resid 270 and name CD2)	(segid 3A4 and resid 276 and name CA)	4.84	0.14	0.14
	assign (segid 3A4 and resid 270 and name CD2)	(segid 3A4 and resid 276 and name CB)	4.17	0.19	0.19
	assign (segid 3A4 and resid 270 and name CD2)	(segid 3A4 and resid 276 and name CG2)	5.44	0.22	0.23
	assign (segid 3A4 and resid 270 and name CD2)	(segid 3A4 and resid 276 and name N)	5.75	0.17	0.18
	assign (segid 3A4 and resid 270 and name CD2)	(segid 3A4 and resid 276 and name O)	4.44	0.20	0.19
70	assign (segid 3A4 and resid 270 and name CD2)	(segid 3A4 and resid 276 and name C)	5.32	0.27	0.27
	assign (segid 3A4 and resid 270 and name CD2)	(segid 3A4 and resid 277 and name CA)	3.99	0.27	0.27
	assign (segid 3A4 and resid 270 and name CD2)	(segid 3A4 and resid 277 and name CB)	4.40	0.34	0.34
	assign (segid 3A4 and resid 270 and name CD2)	(segid 3A4 and resid 277 and name N)	3.91	0.23	0.22
	assign (segid 3A4 and resid 270 and name CD2)	(segid 3A4 and resid 277 and name O)	5.72	0.33	0.32
75	assign (segid 3A4 and resid 270 and name CD2)	(segid 3A4 and resid 278 and name N)	6.28	0.24	0.25
	assign (segid 3A4 and resid 270 and name CD2)	(segid 3A4 and resid 280 and name CA)	6.59	0.55	0.54
	assign (segid 3A4 and resid 270 and name CD2)	(segid 3A4 and resid 280 and name CB)	5.30	0.60	0.61
	assign (segid 3A4 and resid 270 and name CD2)	(segid 3A4 and resid 280 and name N)	6.57	0.45	0.44
80	assign (segid 3A4 and resid 270 and name CD2)	(segid 3A4 and resid 308 and name CB)	5.91	0.66	0.66
	assign (segid 3A4 and resid 270 and name CD2)	(segid 3A4 and resid 308 and name O)	7.39	0.36	0.37
	assign (segid 3A4 and resid 270 and name CD2)	(segid 3A4 and resid 363 and name CG)	7.09	0.42	0.42
	assign (segid 3A4 and resid 270 and name CD2)	(segid 3A4 and resid 409 and name CD2)	6.16	0.50	0.51

	assign (segid 3A4 and resid 270 and name CD2)	(segid 3A4 and resid 409 and name CG)	6.47	0.33	0.34
	assign (segid 3A4 and resid 270 and name CG)	(segid 3A4 and resid 270 and name CD1)	1.51	0.00	0.01
	assign (segid 3A4 and resid 270 and name CG)	(segid 3A4 and resid 270 and name CD2)	1.51	0.02	0.01
	assign (segid 3A4 and resid 270 and name CG)	(segid 3A4 and resid 271 and name C)	6.83	0.03	0.03
5	assign (segid 3A4 and resid 270 and name CG)	(segid 3A4 and resid 271 and name CA)	6.01	0.08	0.08
	assign (segid 3A4 and resid 270 and name CG)	(segid 3A4 and resid 271 and name CB)	6.84	0.15	0.14
	assign (segid 3A4 and resid 270 and name CG)	(segid 3A4 and resid 271 and name N)	4.66	0.05	0.05
	assign (segid 3A4 and resid 270 and name CG)	(segid 3A4 and resid 271 and name O)	7.78	0.09	0.09
	assign (segid 3A4 and resid 270 and name CG)	(segid 3A4 and resid 272 and name C)	7.80	0.07	0.08
	assign (segid 3A4 and resid 270 and name CG)	(segid 3A4 and resid 272 and name N)	6.78	0.05	0.05
10	assign (segid 3A4 and resid 270 and name CG)	(segid 3A4 and resid 272 and name O)	6.64	0.15	0.15
	assign (segid 3A4 and resid 270 and name CG)	(segid 3A4 and resid 273 and name C)	7.04	0.09	0.09
	assign (segid 3A4 and resid 270 and name CG)	(segid 3A4 and resid 273 and name CA)	6.76	0.18	0.18
	assign (segid 3A4 and resid 270 and name CG)	(segid 3A4 and resid 273 and name CB)	6.74	0.06	0.07
	assign (segid 3A4 and resid 270 and name CG)	(segid 3A4 and resid 273 and name N)	5.93	0.15	0.15
15	assign (segid 3A4 and resid 270 and name CG)	(segid 3A4 and resid 273 and name O)	7.46	0.27	0.28
	assign (segid 3A4 and resid 270 and name CG)	(segid 3A4 and resid 274 and name N)	5.54	0.16	0.16
	assign (segid 3A4 and resid 270 and name CG)	(segid 3A4 and resid 276 and name C)	6.25	0.15	0.14
	assign (segid 3A4 and resid 270 and name CG)	(segid 3A4 and resid 276 and name CA)	5.53	0.16	0.16
	assign (segid 3A4 and resid 270 and name CG)	(segid 3A4 and resid 276 and name CB)	6.73	0.18	0.18
20	assign (segid 3A4 and resid 270 and name CG)	(segid 3A4 and resid 276 and name CG2)	7.04	0.17	0.17
	assign (segid 3A4 and resid 270 and name CG)	(segid 3A4 and resid 276 and name N)	5.83	0.19	0.19
	assign (segid 3A4 and resid 270 and name CG)	(segid 3A4 and resid 276 and name O)	6.26	0.25	0.25
	assign (segid 3A4 and resid 270 and name CG)	(segid 3A4 and resid 277 and name C)	4.91	0.24	0.24
	assign (segid 3A4 and resid 270 and name CG)	(segid 3A4 and resid 277 and name CA)	4.94	0.32	0.32
25	assign (segid 3A4 and resid 270 and name CG)	(segid 3A4 and resid 277 and name CB)	5.08	0.21	0.21
	assign (segid 3A4 and resid 270 and name CG)	(segid 3A4 and resid 277 and name N)	6.57	0.30	0.30
	assign (segid 3A4 and resid 270 and name CG)	(segid 3A4 and resid 277 and name O)	7.30	0.24	0.23
	assign (segid 3A4 and resid 270 and name CG)	(segid 3A4 and resid 278 and name N)	6.22	0.56	0.56
30	assign (segid 3A4 and resid 270 and name CG)	(segid 3A4 and resid 280 and name CB)	7.43	0.27	0.28
	assign (segid 3A4 and resid 270 and name CG)	(segid 3A4 and resid 409 and name CB)	5.72	0.41	0.41
	assign (segid 3A4 and resid 270 and name CG)	(segid 3A4 and resid 409 and name CD2)	6.11	0.29	0.30
	assign (segid 3A4 and resid 270 and name CG)	(segid 3A4 and resid 409 and name CG)	2.45	0.02	0.02
	assign (segid 3A4 and resid 270 and name N)	(segid 3A4 and resid 270 and name C)	1.46	0.02	0.02
35	assign (segid 3A4 and resid 270 and name N)	(segid 3A4 and resid 270 and name CA)	2.45	0.02	0.02
	assign (segid 3A4 and resid 270 and name N)	(segid 3A4 and resid 270 and name CB)	4.39	0.07	0.06
	assign (segid 3A4 and resid 270 and name N)	(segid 3A4 and resid 270 and name CD1)	3.82	0.07	0.07
	assign (segid 3A4 and resid 270 and name N)	(segid 3A4 and resid 270 and name CD2)	3.09	0.03	0.03
	assign (segid 3A4 and resid 270 and name N)	(segid 3A4 and resid 270 and name CG)	3.51	0.04	0.04
40	assign (segid 3A4 and resid 270 and name N)	(segid 3A4 and resid 270 and name O)	4.68	0.08	0.07
	assign (segid 3A4 and resid 270 and name N)	(segid 3A4 and resid 271 and name C)	4.19	0.06	0.06
	assign (segid 3A4 and resid 270 and name N)	(segid 3A4 and resid 271 and name CA)	4.92	0.09	0.09
	assign (segid 3A4 and resid 270 and name N)	(segid 3A4 and resid 271 and name CB)	2.77	0.06	0.07
	assign (segid 3A4 and resid 270 and name N)	(segid 3A4 and resid 271 and name N)	5.82	0.12	0.11
	assign (segid 3A4 and resid 270 and name N)	(segid 3A4 and resid 271 and name O)	5.49	0.06	0.05
45	assign (segid 3A4 and resid 270 and name N)	(segid 3A4 and resid 272 and name C)	5.23	0.11	0.11
	assign (segid 3A4 and resid 270 and name N)	(segid 3A4 and resid 272 and name CA)	5.41	0.22	0.22
	assign (segid 3A4 and resid 270 and name N)	(segid 3A4 and resid 272 and name CB)	4.22	0.09	0.09
	assign (segid 3A4 and resid 270 and name N)	(segid 3A4 and resid 272 and name N)	6.65	0.05	0.05
	assign (segid 3A4 and resid 270 and name N)	(segid 3A4 and resid 272 and name O)	5.73	0.21	0.21
50	assign (segid 3A4 and resid 270 and name N)	(segid 3A4 and resid 273 and name C)	5.53	0.12	0.11
	assign (segid 3A4 and resid 270 and name N)	(segid 3A4 and resid 273 and name CA)	5.33	0.19	0.19
	assign (segid 3A4 and resid 270 and name N)	(segid 3A4 and resid 273 and name CB)	4.75	0.10	0.11
	assign (segid 3A4 and resid 270 and name N)	(segid 3A4 and resid 273 and name N)	5.54	0.24	0.23
	assign (segid 3A4 and resid 270 and name N)	(segid 3A4 and resid 273 and name O)	6.62	0.32	0.31
55	assign (segid 3A4 and resid 270 and name N)	(segid 3A4 and resid 274 and name N)	7.05	0.24	0.24
	assign (segid 3A4 and resid 270 and name N)	(segid 3A4 and resid 276 and name C)	7.23	0.22	0.22
	assign (segid 3A4 and resid 270 and name N)	(segid 3A4 and resid 276 and name CA)	6.19	0.22	0.22
	assign (segid 3A4 and resid 270 and name N)	(segid 3A4 and resid 276 and name CB)	6.93	0.21	0.20
	assign (segid 3A4 and resid 270 and name N)	(segid 3A4 and resid 276 and name CG2)	6.70	0.31	0.32
60	assign (segid 3A4 and resid 270 and name N)	(segid 3A4 and resid 277 and name CA)	6.70	0.31	0.32
	assign (segid 3A4 and resid 270 and name N)	(segid 3A4 and resid 277 and name CB)	6.33	0.41	0.40
	assign (segid 3A4 and resid 270 and name N)	(segid 3A4 and resid 277 and name N)	6.45	0.26	0.26
	assign (segid 3A4 and resid 270 and name N)	(segid 3A4 and resid 277 and name O)	3.20	0.05	0.04
	assign (segid 3A4 and resid 270 and name O)	(segid 3A4 and resid 270 and name CD1)	5.55	0.10	0.09
65	assign (segid 3A4 and resid 270 and name O)	(segid 3A4 and resid 270 and name CD2)	4.59	0.08	0.07
	assign (segid 3A4 and resid 270 and name O)	(segid 3A4 and resid 270 and name CG)	4.47	0.04	0.05
	assign (segid 3A4 and resid 270 and name O)	(segid 3A4 and resid 271 and name C)	3.03	0.09	0.09
	assign (segid 3A4 and resid 270 and name O)	(segid 3A4 and resid 271 and name CA)	2.77	0.05	0.05
	assign (segid 3A4 and resid 270 and name O)	(segid 3A4 and resid 271 and name CB)	4.24	0.05	0.04
70	assign (segid 3A4 and resid 270 and name O)	(segid 3A4 and resid 271 and name N)	2.25	0.03	0.03
	assign (segid 3A4 and resid 270 and name O)	(segid 3A4 and resid 271 and name O)	3.60	0.13	0.13
	assign (segid 3A4 and resid 270 and name O)	(segid 3A4 and resid 272 and name C)	4.23	0.17	0.17
	assign (segid 3A4 and resid 270 and name O)	(segid 3A4 and resid 272 and name CA)	4.40	0.16	0.16
	assign (segid 3A4 and resid 270 and name O)	(segid 3A4 and resid 272 and name CB)	5.50	0.11	0.10
75	assign (segid 3A4 and resid 270 and name O)	(segid 3A4 and resid 272 and name N)	3.41	0.14	0.15
	assign (segid 3A4 and resid 270 and name O)	(segid 3A4 and resid 272 and name O)	5.31	0.13	0.14
	assign (segid 3A4 and resid 270 and name O)	(segid 3A4 and resid 273 and name C)	3.43	0.14	0.14
	assign (segid 3A4 and resid 270 and name O)	(segid 3A4 and resid 273 and name CA)	3.92	0.15	0.14
	assign (segid 3A4 and resid 270 and name O)	(segid 3A4 and resid 273 and name CB)	4.62	0.23	0.22
80	assign (segid 3A4 and resid 270 and name O)	(segid 3A4 and resid 273 and name N)	3.30	0.19	0.19
	assign (segid 3A4 and resid 270 and name O)	(segid 3A4 and resid 273 and name O)	3.50	0.15	0.14
	assign (segid 3A4 and resid 270 and name O)	(segid 3A4 and resid 274 and name C)	5.08	0.33	0.33
	assign (segid 3A4 and resid 270 and name O)	(segid 3A4 and resid 274 and name CA)	4.13	0.45	0.46

	assign (segid 3A4 and resid 270 and name O) (segid 3A4 and resid 274 and name CB)	5.14	0.61	0.60
	assign (segid 3A4 and resid 270 and name O) (segid 3A4 and resid 271 and name N)	3.75	0.30	0.30
	assign (segid 3A4 and resid 270 and name O) (segid 3A4 and resid 274 and name O)	5.45	0.32	0.32
	assign (segid 3A4 and resid 270 and name O) (segid 3A4 and resid 275 and name C)	6.85	0.25	0.24
5	assign (segid 3A4 and resid 270 and name O) (segid 3A4 and resid 275 and name CA)	7.01	0.27	0.27
	assign (segid 3A4 and resid 270 and name O) (segid 3A4 and resid 275 and name N)	5.86	0.31	0.31
	assign (segid 3A4 and resid 270 and name O) (segid 3A4 and resid 276 and name C)	5.87	0.27	0.27
	assign (segid 3A4 and resid 270 and name O) (segid 3A4 and resid 276 and name CA)	6.18	0.22	0.21
	assign (segid 3A4 and resid 270 and name O) (segid 3A4 and resid 276 and name CB)	5.77	0.19	0.19
	assign (segid 3A4 and resid 270 and name O) (segid 3A4 and resid 276 and name CG2)	6.67	0.23	0.24
10	assign (segid 3A4 and resid 270 and name O) (segid 3A4 and resid 276 and name N)	5.98	0.22	0.21
	assign (segid 3A4 and resid 270 and name O) (segid 3A4 and resid 276 and name O)	6.83	0.29	0.30
	assign (segid 3A4 and resid 270 and name O) (segid 3A4 and resid 277 and name C)	6.33	0.42	0.42
	assign (segid 3A4 and resid 270 and name O) (segid 3A4 and resid 277 and name CA)	4.98	0.41	0.41
	assign (segid 3A4 and resid 270 and name O) (segid 3A4 and resid 277 and name CB)	4.06	0.51	0.51
15	assign (segid 3A4 and resid 270 and name O) (segid 3A4 and resid 277 and name N)	4.81	0.33	0.33
	assign (segid 3A4 and resid 270 and name O) (segid 3A4 and resid 277 and name O)	7.22	0.45	0.45
	assign (segid 3A4 and resid 270 and name O) (segid 3A4 and resid 278 and name N)	6.73	0.38	0.38
	assign (segid 3A4 and resid 270 and name O) (segid 3A4 and resid 271 and name CB)	2.51	0.04	0.03
20	assign (segid 3A4 and resid 271 and name C) (segid 3A4 and resid 271 and name O)	1.24	0.03	0.03
	assign (segid 3A4 and resid 271 and name C) (segid 3A4 and resid 272 and name C)	3.19	0.08	0.08
	assign (segid 3A4 and resid 271 and name C) (segid 3A4 and resid 272 and name CA)	2.42	0.02	0.03
	assign (segid 3A4 and resid 271 and name C) (segid 3A4 and resid 272 and name CB)	3.66	0.03	0.03
	assign (segid 3A4 and resid 271 and name C) (segid 3A4 and resid 272 and name N)	1.32	0.01	0.01
25	assign (segid 3A4 and resid 271 and name C) (segid 3A4 and resid 272 and name O)	4.23	0.14	0.14
	assign (segid 3A4 and resid 271 and name C) (segid 3A4 and resid 273 and name C)	4.87	0.18	0.18
	assign (segid 3A4 and resid 271 and name C) (segid 3A4 and resid 273 and name CA)	4.62	0.10	0.10
	assign (segid 3A4 and resid 271 and name C) (segid 3A4 and resid 273 and name CB)	5.64	0.06	0.06
	assign (segid 3A4 and resid 271 and name C) (segid 3A4 and resid 273 and name N)	3.32	0.07	0.07
	assign (segid 3A4 and resid 271 and name C) (segid 3A4 and resid 273 and name O)	5.59	0.18	0.17
30	assign (segid 3A4 and resid 271 and name C) (segid 3A4 and resid 274 and name C)	6.98	0.27	0.28
	assign (segid 3A4 and resid 271 and name C) (segid 3A4 and resid 274 and name CA)	5.64	0.33	0.34
	assign (segid 3A4 and resid 271 and name C) (segid 3A4 and resid 274 and name CB)	6.03	0.47	0.46
	assign (segid 3A4 and resid 271 and name C) (segid 3A4 and resid 274 and name N)	4.86	0.28	0.28
	assign (segid 3A4 and resid 271 and name C) (segid 3A4 and resid 277 and name CB)	6.86	0.54	0.53
35	assign (segid 3A4 and resid 271 and name C) (segid 3A4 and resid 271 and name C)	1.51	0.01	0.01
	assign (segid 3A4 and resid 271 and name CA) (segid 3A4 and resid 271 and name CB)	1.52	0.01	0.01
	assign (segid 3A4 and resid 271 and name CA) (segid 3A4 and resid 271 and name O)	2.40	0.03	0.03
	assign (segid 3A4 and resid 271 and name CA) (segid 3A4 and resid 272 and name C)	4.53	0.08	0.07
	assign (segid 3A4 and resid 271 and name CA) (segid 3A4 and resid 272 and name CA)	3.78	0.02	0.02
40	assign (segid 3A4 and resid 271 and name CA) (segid 3A4 and resid 272 and name CB)	4.81	0.03	0.02
	assign (segid 3A4 and resid 271 and name CA) (segid 3A4 and resid 272 and name N)	2.41	0.01	0.02
	assign (segid 3A4 and resid 271 and name CA) (segid 3A4 and resid 272 and name O)	5.64	0.12	0.13
	assign (segid 3A4 and resid 271 and name CA) (segid 3A4 and resid 273 and name C)	5.56	0.21	0.20
45	assign (segid 3A4 and resid 271 and name CA) (segid 3A4 and resid 273 and name CA)	5.57	0.11	0.11
	assign (segid 3A4 and resid 271 and name CA) (segid 3A4 and resid 273 and name CB)	6.43	0.09	0.10
	assign (segid 3A4 and resid 271 and name CA) (segid 3A4 and resid 273 and name N)	4.37	0.08	0.07
	assign (segid 3A4 and resid 271 and name CA) (segid 3A4 and resid 273 and name O)	6.01	0.19	0.20
	assign (segid 3A4 and resid 271 and name CA) (segid 3A4 and resid 274 and name CA)	6.11	0.45	0.44
	assign (segid 3A4 and resid 271 and name CA) (segid 3A4 and resid 274 and name CB)	6.60	0.64	0.64
50	assign (segid 3A4 and resid 271 and name CA) (segid 3A4 and resid 274 and name N)	5.59	0.35	0.35
	assign (segid 3A4 and resid 271 and name CA) (segid 3A4 and resid 275 and name CA)	9.47	0.31	0.31
	assign (segid 3A4 and resid 271 and name CA) (segid 3A4 and resid 275 and name CB)	10.40	0.29	0.29
	assign (segid 3A4 and resid 271 and name CA) (segid 3A4 and resid 276 and name CA)	8.92	0.24	0.24
	assign (segid 3A4 and resid 271 and name CA) (segid 3A4 and resid 276 and name CB)	8.40	0.21	0.21
55	assign (segid 3A4 and resid 271 and name CA) (segid 3A4 and resid 276 and name N)	7.48	0.46	0.47
	assign (segid 3A4 and resid 271 and name CA) (segid 3A4 and resid 277 and name CB)	6.34	0.56	0.55
	assign (segid 3A4 and resid 271 and name CA) (segid 3A4 and resid 278 and name CA)	10.49	0.48	0.47
	assign (segid 3A4 and resid 271 and name CA) (segid 3A4 and resid 278 and name CB)	10.90	0.48	0.48
	assign (segid 3A4 and resid 271 and name CA) (segid 3A4 and resid 279 and name CA)	12.76	0.41	0.41
60	assign (segid 3A4 and resid 271 and name CA) (segid 3A4 and resid 279 and name CB)	12.77	0.36	0.36
	assign (segid 3A4 and resid 271 and name CA) (segid 3A4 and resid 280 and name CA)	12.21	0.59	0.59
	assign (segid 3A4 and resid 271 and name CA) (segid 3A4 and resid 280 and name CB)	11.13	0.64	0.64
	assign (segid 3A4 and resid 271 and name CA) (segid 3A4 and resid 281 and name CA)	12.84	0.79	0.79
65	assign (segid 3A4 and resid 271 and name CA) (segid 3A4 and resid 281 and name CB)	12.15	0.78	0.78
	assign (segid 3A4 and resid 271 and name CA) (segid 3A4 and resid 282 and name CA)	15.82	0.71	0.71
	assign (segid 3A4 and resid 271 and name CA) (segid 3A4 and resid 304 and name CA)	16.71	0.71	0.70
	assign (segid 3A4 and resid 271 and name CA) (segid 3A4 and resid 304 and name CB)	16.03	0.71	0.71
	assign (segid 3A4 and resid 271 and name CA) (segid 3A4 and resid 305 and name CA)	15.11	0.68	0.68
	assign (segid 3A4 and resid 271 and name CA) (segid 3A4 and resid 305 and name CB)	15.38	0.65	0.65
70	assign (segid 3A4 and resid 271 and name CA) (segid 3A4 and resid 306 and name CA)	17.68	0.64	0.64
	assign (segid 3A4 and resid 271 and name CA) (segid 3A4 and resid 307 and name CA)	16.98	0.77	0.78
	assign (segid 3A4 and resid 271 and name CA) (segid 3A4 and resid 307 and name CB)	17.23	0.84	0.85
	assign (segid 3A4 and resid 271 and name CA) (segid 3A4 and resid 308 and name CA)	13.28	0.75	0.76
	assign (segid 3A4 and resid 271 and name CA) (segid 3A4 and resid 308 and name CB)	12.35	0.79	0.78
75	assign (segid 3A4 and resid 271 and name CA) (segid 3A4 and resid 309 and name CA)	14.53	0.56	0.56
	assign (segid 3A4 and resid 271 and name CA) (segid 3A4 and resid 309 and name CB)	15.51	0.60	0.59
	assign (segid 3A4 and resid 271 and name CA) (segid 3A4 and resid 310 and name CA)	17.11	0.50	0.50
	assign (segid 3A4 and resid 271 and name CA) (segid 3A4 and resid 310 and name CB)	18.17	0.56	0.56
	assign (segid 3A4 and resid 271 and name CA) (segid 3A4 and resid 311 and name CA)	14.94	0.57	0.58
80	assign (segid 3A4 and resid 271 and name CA) (segid 3A4 and resid 311 and name CB)	14.29	0.68	0.69
	assign (segid 3A4 and resid 271 and name CA) (segid 3A4 and resid 312 and name CA)	12.76	0.37	0.36
	assign (segid 3A4 and resid 271 and name CA) (segid 3A4 and resid 312 and name CB)	12.08	0.30	0.29

	assign (segid 3A4 and resid 271 and name CA)	(segid 3A4 and resid 313 and name CA)	16.18	0.27	0.26
	assign (segid 3A4 and resid 271 and name CA)	(segid 3A4 and resid 313 and name CB)	17.25	0.26	0.26
	assign (segid 3A4 and resid 271 and name CA)	(segid 3A4 and resid 314 and name CA)	17.46	0.36	0.36
	assign (segid 3A4 and resid 271 and name CA)	(segid 3A4 and resid 314 and name CB)	17.70	0.45	0.45
	assign (segid 3A4 and resid 271 and name CA)	(segid 3A4 and resid 315 and name CA)	14.90	0.43	0.44
5	assign (segid 3A4 and resid 271 and name CA)	(segid 3A4 and resid 315 and name CB)	13.59	0.48	0.48
	assign (segid 3A4 and resid 271 and name CA)	(segid 3A4 and resid 316 and name CA)	14.68	0.44	0.45
	assign (segid 3A4 and resid 271 and name CA)	(segid 3A4 and resid 317 and name CA)	18.13	0.25	0.25
	assign (segid 3A4 and resid 271 and name CA)	(segid 3A4 and resid 318 and name CA)	18.58	0.22	0.23
	assign (segid 3A4 and resid 271 and name CA)	(segid 3A4 and resid 318 and name CB)	18.08	0.29	0.29
10	assign (segid 3A4 and resid 271 and name CA)	(segid 3A4 and resid 360 and name CA)	19.20	0.52	0.52
	assign (segid 3A4 and resid 271 and name CA)	(segid 3A4 and resid 361 and name CA)	16.64	0.58	0.59
	assign (segid 3A4 and resid 271 and name CA)	(segid 3A4 and resid 361 and name CB)	17.14	0.68	0.67
	assign (segid 3A4 and resid 271 and name CA)	(segid 3A4 and resid 362 and name CA)	14.57	0.73	0.73
	assign (segid 3A4 and resid 271 and name CA)	(segid 3A4 and resid 362 and name CB)	15.33	0.87	0.86
15	assign (segid 3A4 and resid 271 and name CA)	(segid 3A4 and resid 363 and name CA)	12.03	0.78	0.78
	assign (segid 3A4 and resid 271 and name CA)	(segid 3A4 and resid 363 and name CB)	10.58	0.78	0.78
	assign (segid 3A4 and resid 271 and name CA)	(segid 3A4 and resid 364 and name CA)	13.75	0.93	0.93
	assign (segid 3A4 and resid 271 and name CA)	(segid 3A4 and resid 364 and name CB)	15.00	0.95	0.95
	assign (segid 3A4 and resid 271 and name CA)	(segid 3A4 and resid 365 and name CA)	14.10	0.92	0.92
20	assign (segid 3A4 and resid 271 and name CA)	(segid 3A4 and resid 365 and name CB)	13.27	0.94	0.95
	assign (segid 3A4 and resid 271 and name CA)	(segid 3A4 and resid 401 and name CA)	16.25	0.53	0.53
	assign (segid 3A4 and resid 271 and name CA)	(segid 3A4 and resid 402 and name CA)	16.81	0.56	0.56
	assign (segid 3A4 and resid 271 and name CA)	(segid 3A4 and resid 402 and name CB)	18.05	0.55	0.55
	assign (segid 3A4 and resid 271 and name CA)	(segid 3A4 and resid 403 and name CA)	18.09	0.69	0.69
25	assign (segid 3A4 and resid 271 and name CA)	(segid 3A4 and resid 404 and name CA)	15.39	0.84	0.85
	assign (segid 3A4 and resid 271 and name CA)	(segid 3A4 and resid 404 and name CB)	15.10	0.89	0.88
	assign (segid 3A4 and resid 271 and name CA)	(segid 3A4 and resid 405 and name CA)	12.58	0.73	0.73
	assign (segid 3A4 and resid 271 and name CA)	(segid 3A4 and resid 405 and name CB)	12.23	0.67	0.67
	assign (segid 3A4 and resid 271 and name CA)	(segid 3A4 and resid 406 and name CA)	14.84	0.90	0.90
30	assign (segid 3A4 and resid 271 and name CA)	(segid 3A4 and resid 407 and name CA)	15.71	0.79	0.80
	assign (segid 3A4 and resid 271 and name CA)	(segid 3A4 and resid 407 and name CB)	16.70	0.76	0.76
	assign (segid 3A4 and resid 271 and name CA)	(segid 3A4 and resid 408 and name CA)	12.53	0.76	0.77
	assign (segid 3A4 and resid 271 and name CA)	(segid 3A4 and resid 408 and name CB)	11.53	0.79	0.78
	assign (segid 3A4 and resid 271 and name CA)	(segid 3A4 and resid 409 and name CA)	11.11	0.71	0.71
35	assign (segid 3A4 and resid 271 and name CA)	(segid 3A4 and resid 409 and name CB)	10.64	0.82	0.83
	assign (segid 3A4 and resid 271 and name CA)	(segid 3A4 and resid 410 and name CA)	14.57	0.67	0.67
	assign (segid 3A4 and resid 271 and name CA)	(segid 3A4 and resid 411 and name CA)	14.95	0.60	0.60
	assign (segid 3A4 and resid 271 and name CA)	(segid 3A4 and resid 411 and name CB)	15.38	0.59	0.60
	assign (segid 3A4 and resid 271 and name CA)	(segid 3A4 and resid 412 and name CA)	11.93	0.65	0.65
40	assign (segid 3A4 and resid 271 and name CA)	(segid 3A4 and resid 413 and name CA)	9.15	1.42	1.41
	assign (segid 3A4 and resid 271 and name CA)	(segid 3A4 and resid 414 and name C)	6.12	0.92	0.92
	assign (segid 3A4 and resid 271 and name CA)	(segid 3A4 and resid 414 and name CA)	6.78	1.24	1.23
	assign (segid 3A4 and resid 271 and name CA)	(segid 3A4 and resid 414 and name O)	5.68	0.77	0.78
	assign (segid 3A4 and resid 271 and name CA)	(segid 3A4 and resid 415 and name C)	6.58	0.60	0.60
45	assign (segid 3A4 and resid 271 and name CA)	(segid 3A4 and resid 415 and name CA)	6.24	0.74	0.73
	assign (segid 3A4 and resid 271 and name CA)	(segid 3A4 and resid 415 and name CB)	7.11	0.91	0.91
	assign (segid 3A4 and resid 271 and name CA)	(segid 3A4 and resid 415 and name N)	6.38	0.91	0.91
	assign (segid 3A4 and resid 271 and name CA)	(segid 3A4 and resid 416 and name CA)	7.00	0.97	0.98
	assign (segid 3A4 and resid 271 and name CA)	(segid 3A4 and resid 417 and name CA)	10.40	0.60	0.61
50	assign (segid 3A4 and resid 271 and name CA)	(segid 3A4 and resid 423 and name CA)	11.84	1.12	1.11
	assign (segid 3A4 and resid 271 and name CA)	(segid 3A4 and resid 424 and name CA)	11.57	0.88	0.88
	assign (segid 3A4 and resid 271 and name CA)	(segid 3A4 and resid 425 and name CA)	13.65	1.12	1.12
	assign (segid 3A4 and resid 271 and name CA)	(segid 3A4 and resid 426 and name CA)	15.39	0.45	0.45
	assign (segid 3A4 and resid 271 and name CA)	(segid 3A4 and resid 427 and name CA)	17.82	1.13	1.12
55	assign (segid 3A4 and resid 271 and name CA)	(segid 3A4 and resid 433 and name CA)	18.56	0.74	0.75
	assign (segid 3A4 and resid 271 and name CA)	(segid 3A4 and resid 434 and name CA)	15.93	0.39	0.40
	assign (segid 3A4 and resid 271 and name CA)	(segid 3A4 and resid 435 and name CA)	13.57	0.29	0.29
	assign (segid 3A4 and resid 271 and name CA)	(segid 3A4 and resid 436 and name CA)	15.46	0.97	0.98
	assign (segid 3A4 and resid 271 and name CA)	(segid 3A4 and resid 437 and name CA)	13.98	0.60	0.61
60	assign (segid 3A4 and resid 271 and name CA)	(segid 3A4 and resid 438 and name CA)	10.55	0.50	0.50
	assign (segid 3A4 and resid 271 and name CA)	(segid 3A4 and resid 439 and name CA)	10.91	0.57	0.57
	assign (segid 3A4 and resid 271 and name CA)	(segid 3A4 and resid 440 and name CA)	8.89	0.76	0.77
	assign (segid 3A4 and resid 271 and name CA)	(segid 3A4 and resid 272 and name C)	5.57	0.11	0.10
	assign (segid 3A4 and resid 271 and name CA)	(segid 3A4 and resid 272 and name CA)	4.50	0.09	0.09
65	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 272 and name CB)	5.25	0.07	0.08
	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 272 and name N)	3.20	0.08	0.08
	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 272 and name O)	6.63	0.16	0.16
	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 273 and name C)	7.04	0.20	0.20
	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 273 and name CA)	6.93	0.11	0.11
70	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 273 and name CB)	7.75	0.09	0.09
	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 273 and name N)	5.63	0.09	0.10
	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 274 and name CA)	7.57	0.44	0.43
	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 274 and name CB)	7.95	0.64	0.63
	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 274 and name N)	7.06	0.34	0.33
75	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 275 and name CA)	10.98	0.31	0.30
	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 275 and name CB)	11.90	0.28	0.28
	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 276 and name CA)	10.37	0.25	0.25
	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 276 and name CB)	9.79	0.21	0.22
80	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 277 and name CA)	8.79	0.49	0.49
	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 277 and name CB)	7.62	0.57	0.57
	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 278 and name CA)	11.82	0.51	0.51
	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 278 and name CB)	12.28	0.51	0.50

	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 279 and name CA)	14.13	0.44	0.45
	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 279 and name CB)	14.18	0.38	0.38
	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 280 and name CA)	13.36	0.66	0.66
	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 280 and name CB)	12.22	0.72	0.71
5	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 281 and name CA)	13.87	0.91	0.90
	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 281 and name CB)	13.17	0.89	0.88
	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 282 and name CA)	17.00	0.81	0.81
	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 304 and name CA)	17.79	0.77	0.77
	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 304 and name CB)	17.19	0.77	0.77
10	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 305 and name CA)	15.96	0.79	0.78
	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 305 and name CB)	16.15	0.77	0.77
	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 306 and name CA)	18.43	0.73	0.73
	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 307 and name CA)	17.90	0.83	0.83
	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 308 and name CA)	14.15	0.82	0.83
15	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 308 and name CB)	13.24	0.86	0.87
	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 309 and name CA)	15.06	0.64	0.64
	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 309 and name CB)	15.98	0.68	0.68
	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 310 and name CA)	17.71	0.56	0.56
	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 311 and name CA)	15.65	0.63	0.63
20	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 311 and name CB)	15.12	0.72	0.73
	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 312 and name CA)	13.17	0.45	0.45
	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 312 and name CB)	12.43	0.38	0.38
	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 313 and name CA)	16.40	0.32	0.31
	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 313 and name CB)	17.49	0.31	0.30
25	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 314 and name CA)	17.86	0.41	0.41
	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 314 and name CB)	18.21	0.50	0.50
	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 315 and name CA)	15.25	0.48	0.48
	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 315 and name CB)	14.01	0.53	0.54
30	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 316 and name CA)	14.66	0.44	0.45
	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 317 and name CA)	18.05	0.24	0.25
	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 318 and name CA)	18.22	0.25	0.25
	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 318 and name CB)	17.69	0.33	0.32
	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 361 and name CA)	17.22	0.63	0.63
	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 361 and name CB)	17.65	0.71	0.72
35	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 362 and name CA)	15.42	0.78	0.77
	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 362 and name CB)	16.27	0.89	0.89
	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 363 and name CA)	12.94	0.83	0.82
	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 363 and name CB)	11.46	0.83	0.83
	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 364 and name CA)	14.90	0.94	0.95
40	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 364 and name CB)	16.16	0.97	0.97
	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 365 and name CA)	15.24	0.94	0.95
	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 365 and name CB)	14.44	0.97	0.98
	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 401 and name CA)	16.27	0.56	0.57
	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 402 and name CA)	17.12	0.63	0.64
45	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 402 and name CB)	18.43	0.63	0.63
	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 403 and name CA)	18.24	0.75	0.75
	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 404 and name CA)	15.32	0.87	0.87
	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 404 and name CB)	14.92	0.87	0.87
	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 405 and name CA)	12.79	0.81	0.81
50	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 405 and name CB)	12.53	0.76	0.76
	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 406 and name CA)	15.26	0.99	0.99
	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 407 and name CA)	15.86	0.90	0.89
	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 407 and name CB)	16.74	0.86	0.86
	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 408 and name CA)	12.51	0.88	0.88
55	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 408 and name CB)	11.42	0.88	0.89
	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 409 and name CA)	11.49	0.82	0.83
	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 409 and name CB)	11.18	0.92	0.92
	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 410 and name CA)	14.99	0.76	0.76
	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 411 and name CA)	15.04	0.65	0.65
60	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 411 and name CB)	15.35	0.63	0.64
	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 412 and name CA)	11.96	0.62	0.62
	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 413 and name CA)	9.29	1.40	1.40
	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 414 and name C)	5.76	0.96	0.96
	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 414 and name CA)	6.50	1.22	1.23
65	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 414 and name O)	5.52	0.73	0.74
	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 415 and name C)	5.65	0.64	0.64
	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 415 and name CA)	5.56	0.81	0.81
	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 415 and name CB)	6.53	1.01	1.01
	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 415 and name N)	5.79	0.98	0.98
70	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 415 and name O)	6.32	0.62	0.62
	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 416 and name CA)	5.87	0.98	0.97
	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 416 and name N)	5.34	0.78	0.77
	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 417 and name CA)	9.31	0.68	0.68
75	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 423 and name CA)	10.77	1.05	1.04
	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 424 and name CA)	10.56	0.83	0.83
	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 425 and name CA)	12.64	1.03	1.03
	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 426 and name CA)	14.44	0.50	0.50
	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 427 and name CA)	16.88	1.08	1.08
80	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 433 and name CA)	17.88	0.70	0.71
	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 434 and name CA)	15.09	0.40	0.40
	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 435 and name CA)	12.54	0.23	0.24
	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 436 and name CA)	14.24	0.93	0.93
	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 437 and name CA)	12.59	0.60	0.59

	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 438 and name CA)	9.11	0.50	0.50
	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 439 and name CA)	9.42	0.59	0.58
	assign (segid 3A4 and resid 271 and name CB)	(segid 3A4 and resid 440 and name CA)	7.58	0.80	0.79
	assign (segid 3A4 and resid 271 and name N)	(segid 3A4 and resid 271 and name C)	2.41	0.03	0.03
5	assign (segid 3A4 and resid 271 and name N)	(segid 3A4 and resid 271 and name CA)	1.46	0.01	0.01
	assign (segid 3A4 and resid 271 and name N)	(segid 3A4 and resid 271 and name CB)	2.44	0.04	0.03
	assign (segid 3A4 and resid 271 and name N)	(segid 3A4 and resid 271 and name O)	3.50	0.06	0.06
	assign (segid 3A4 and resid 271 and name N)	(segid 3A4 and resid 272 and name C)	4.67	0.07	0.08
	assign (segid 3A4 and resid 271 and name N)	(segid 3A4 and resid 272 and name CA)	4.10	0.06	0.06
10	assign (segid 3A4 and resid 271 and name N)	(segid 3A4 and resid 272 and name CB)	4.88	0.12	0.11
	assign (segid 3A4 and resid 271 and name N)	(segid 3A4 and resid 272 and name N)	2.69	0.06	0.05
	assign (segid 3A4 and resid 271 and name N)	(segid 3A4 and resid 272 and name O)	5.88	0.10	0.10
	assign (segid 3A4 and resid 271 and name N)	(segid 3A4 and resid 273 and name C)	5.32	0.21	0.21
	assign (segid 3A4 and resid 271 and name N)	(segid 3A4 and resid 273 and name CA)	5.32	0.10	0.10
15	assign (segid 3A4 and resid 271 and name N)	(segid 3A4 and resid 273 and name CB)	5.88	0.11	0.11
	assign (segid 3A4 and resid 271 and name N)	(segid 3A4 and resid 273 and name N)	4.21	0.08	0.09
	assign (segid 3A4 and resid 271 and name N)	(segid 3A4 and resid 273 and name O)	5.53	0.20	0.20
	assign (segid 3A4 and resid 271 and name N)	(segid 3A4 and resid 274 and name CA)	6.22	0.46	0.46
	assign (segid 3A4 and resid 271 and name N)	(segid 3A4 and resid 274 and name N)	5.68	0.35	0.34
20	assign (segid 3A4 and resid 271 and name N)	(segid 3A4 and resid 276 and name CB)	7.45	0.19	0.19
	assign (segid 3A4 and resid 271 and name N)	(segid 3A4 and resid 277 and name CA)	6.80	0.43	0.42
	assign (segid 3A4 and resid 271 and name N)	(segid 3A4 and resid 277 and name CB)	5.85	0.51	0.52
	assign (segid 3A4 and resid 271 and name N)	(segid 3A4 and resid 277 and name N)	6.79	0.33	0.33
	assign (segid 3A4 and resid 271 and name N)	(segid 3A4 and resid 414 and name O)	6.59	0.70	0.71
25	assign (segid 3A4 and resid 271 and name O)	(segid 3A4 and resid 271 and name CB)	3.26	0.04	0.05
	assign (segid 3A4 and resid 271 and name O)	(segid 3A4 and resid 272 and name C)	3.27	0.14	0.14
	assign (segid 3A4 and resid 271 and name O)	(segid 3A4 and resid 272 and name CA)	2.75	0.07	0.06
	assign (segid 3A4 and resid 271 and name O)	(segid 3A4 and resid 272 and name CB)	4.17	0.08	0.07
	assign (segid 3A4 and resid 271 and name O)	(segid 3A4 and resid 272 and name N)	2.24	0.03	0.02
30	assign (segid 3A4 and resid 271 and name O)	(segid 3A4 and resid 272 and name O)	4.05	0.23	0.23
	assign (segid 3A4 and resid 271 and name O)	(segid 3A4 and resid 273 and name C)	4.85	0.26	0.26
	assign (segid 3A4 and resid 271 and name O)	(segid 3A4 and resid 273 and name CA)	4.71	0.19	0.18
	assign (segid 3A4 and resid 271 and name O)	(segid 3A4 and resid 273 and name CB)	5.95	0.14	0.13
	assign (segid 3A4 and resid 271 and name O)	(segid 3A4 and resid 273 and name N)	3.56	0.12	0.12
35	assign (segid 3A4 and resid 271 and name O)	(segid 3A4 and resid 273 and name O)	5.72	0.26	0.26
	assign (segid 3A4 and resid 271 and name O)	(segid 3A4 and resid 274 and name C)	6.68	0.35	0.36
	assign (segid 3A4 and resid 271 and name O)	(segid 3A4 and resid 274 and name CA)	5.25	0.39	0.39
	assign (segid 3A4 and resid 271 and name O)	(segid 3A4 and resid 274 and name CB)	5.35	0.49	0.50
	assign (segid 3A4 and resid 271 and name O)	(segid 3A4 and resid 274 and name N)	4.53	0.34	0.35
40	assign (segid 3A4 and resid 271 and name O)	(segid 3A4 and resid 277 and name CB)	7.07	0.61	0.60
	assign (segid 3A4 and resid 271 and name O)	(segid 3A4 and resid 416 and name N)	6.54	0.75	0.76
	assign (segid 3A4 and resid 272 and name C)	(segid 3A4 and resid 272 and name CB)	2.48	0.02	0.02
	assign (segid 3A4 and resid 272 and name C)	(segid 3A4 and resid 272 and name O)	1.23	0.01	0.02
	assign (segid 3A4 and resid 272 and name C)	(segid 3A4 and resid 273 and name C)	3.54	0.03	0.03
45	assign (segid 3A4 and resid 272 and name C)	(segid 3A4 and resid 273 and name CA)	2.43	0.01	0.01
	assign (segid 3A4 and resid 272 and name C)	(segid 3A4 and resid 273 and name CB)	3.38	0.04	0.03
	assign (segid 3A4 and resid 272 and name C)	(segid 3A4 and resid 273 and name N)	1.33	0.01	0.01
	assign (segid 3A4 and resid 272 and name C)	(segid 3A4 and resid 273 and name O)	4.55	0.04	0.04
	assign (segid 3A4 and resid 272 and name C)	(segid 3A4 and resid 274 and name C)	6.34	0.06	0.07
50	assign (segid 3A4 and resid 272 and name C)	(segid 3A4 and resid 274 and name CA)	5.24	0.06	0.07
	assign (segid 3A4 and resid 272 and name C)	(segid 3A4 and resid 274 and name CB)	5.71	0.09	0.09
	assign (segid 3A4 and resid 272 and name C)	(segid 3A4 and resid 274 and name N)	3.88	0.05	0.06
	assign (segid 3A4 and resid 272 and name C)	(segid 3A4 and resid 274 and name O)	7.35	0.10	0.11
	assign (segid 3A4 and resid 272 and name C)	(segid 3A4 and resid 275 and name CA)	7.71	0.08	0.08
55	assign (segid 3A4 and resid 272 and name C)	(segid 3A4 and resid 275 and name N)	6.43	0.05	0.05
	assign (segid 3A4 and resid 272 and name C)	(segid 3A4 and resid 276 and name CB)	7.17	0.14	0.14
	assign (segid 3A4 and resid 272 and name C)	(segid 3A4 and resid 276 and name CG2)	7.20	0.22	0.23
	assign (segid 3A4 and resid 272 and name C)	(segid 3A4 and resid 276 and name N)	7.23	0.12	0.11
	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 272 and name C)	1.51	0.02	0.02
60	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 272 and name CB)	1.53	0.01	0.01
	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 272 and name O)	2.38	0.02	0.02
	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 273 and name C)	4.76	0.04	0.04
	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 273 and name CA)	3.81	0.02	0.02
	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 273 and name CB)	4.62	0.05	0.04
65	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 273 and name N)	2.44	0.02	0.03
	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 273 and name O)	5.67	0.06	0.06
	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 274 and name C)	7.46	0.08	0.08
	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 274 and name CA)	6.24	0.10	0.10
	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 274 and name CB)	6.64	0.13	0.13
70	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 274 and name N)	5.02	0.07	0.07
	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 275 and name CA)	9.04	0.08	0.07
	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 275 and name CB)	9.46	0.13	0.12
	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 275 and name N)	7.72	0.06	0.07
	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 276 and name CA)	8.96	0.12	0.13
75	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 276 and name CB)	8.20	0.13	0.12
	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 277 and name CA)	9.07	0.36	0.36
	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 277 and name CB)	8.26	0.47	0.46
	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 278 and name CA)	11.81	0.26	0.27
	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 278 and name CB)	11.90	0.27	0.21
80	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 279 and name CA)	13.63	0.22	0.22
	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 279 and name CB)	13.29	0.29	0.29
	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 280 and name CA)	13.81	0.35	0.35
	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 280 and name CB)	12.85	0.42	0.43

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	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 281 and name CA)	15.06	0.53	0.53
	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 281 and name CB)	14.46	0.54	0.54
	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 282 and name CA)	17.54	0.40	0.40
	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 304 and name CA)	17.68	0.54	0.53
5	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 304 and name CB)	16.92	0.46	0.47
	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 305 and name CA)	16.61	0.55	0.54
	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 305 and name CB)	17.18	0.49	0.49
	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 307 and name CA)	17.39	0.76	0.77
	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 307 and name CB)	17.52	0.83	0.83
10	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 308 and name CA)	13.84	0.71	0.71
	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 308 and name CB)	13.23	0.72	0.71
	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 309 and name CA)	15.42	0.63	0.63
	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 309 and name CB)	16.64	0.66	0.66
	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 310 and name CA)	17.29	0.58	0.59
15	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 310 and name CB)	18.29	0.64	0.64
	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 311 and name CA)	14.46	0.63	0.63
	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 311 and name CB)	13.72	0.71	0.71
	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 312 and name CA)	12.66	0.46	0.46
	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 312 and name CB)	12.40	0.44	0.44
20	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 313 and name CA)	16.09	0.43	0.44
	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 313 and name CB)	17.36	0.43	0.42
	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 314 and name CA)	16.59	0.44	0.44
	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 314 and name CB)	16.71	0.52	0.52
	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 315 and name CA)	13.55	0.45	0.45
25	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 315 and name CB)	12.18	0.47	0.47
	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 316 and name CA)	13.84	0.47	0.46
	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 317 and name CA)	17.47	0.38	0.38
	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 318 and name CA)	18.42	0.48	0.48
	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 318 and name CB)	18.20	0.41	0.42
30	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 352 and name CA)	19.27	0.40	0.40
	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 352 and name CB)	18.71	0.49	0.48
	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 359 and name CA)	17.31	0.75	0.75
	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 359 and name CB)	16.73	0.80	0.81
	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 360 and name CA)	16.70	0.54	0.53
35	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 360 and name CB)	17.91	0.49	0.48
	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 361 and name CA)	13.83	0.52	0.52
	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 361 and name CB)	14.14	0.57	0.58
	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 362 and name CA)	11.81	0.75	0.74
	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 362 and name CB)	12.53	0.88	0.88
40	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 363 and name CA)	10.00	0.78	0.78
	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 363 and name CB)	8.65	0.81	0.80
	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 364 and name CA)	12.21	0.92	0.92
	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 364 and name CB)	13.23	0.97	0.97
	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 365 and name CA)	13.55	0.78	0.78
45	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 365 and name CB)	13.06	0.74	0.75
	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 401 and name CA)	18.32	0.47	0.48
	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 402 and name CA)	18.96	0.42	0.42
	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 404 and name CA)	18.29	0.75	0.76
	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 404 and name CB)	17.91	0.81	0.81
50	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 405 and name CA)	15.32	0.66	0.65
	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 405 and name CB)	14.69	0.58	0.59
	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 406 and name CA)	17.63	0.81	0.81
	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 408 and name CA)	16.00	0.70	0.69
	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 408 and name CB)	14.96	0.72	0.72
55	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 409 and name CA)	14.39	0.62	0.62
	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 409 and name CB)	13.72	0.68	0.67
	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 410 and name CA)	17.81	0.58	0.59
	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 411 and name CA)	18.50	0.63	0.63
	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 411 and name CB)	19.00	0.60	0.59
60	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 412 and name CA)	15.50	0.77	0.77
	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 413 and name CA)	12.34	1.63	1.63
	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 414 and name CA)	10.04	1.66	1.67
	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 415 and name CA)	8.83	1.11	1.10
	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 415 and name CB)	9.35	1.45	1.46
65	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 416 and name CA)	8.79	0.92	0.92
	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 417 and name CA)	11.67	0.45	0.45
	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 423 and name CA)	11.02	1.38	1.38
	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 424 and name CA)	10.75	1.34	1.35
	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 425 and name CA)	12.92	1.51	1.51
70	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 426 and name CA)	14.67	0.67	0.67
	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 427 and name CA)	17.29	1.20	1.21
	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 434 and name CA)	16.08	0.63	0.62
	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 435 and name CA)	13.91	0.74	0.74
	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 436 and name CA)	16.07	1.51	1.51
75	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 437 and name CA)	15.08	0.86	0.87
	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 438 and name CA)	12.07	0.64	0.63
	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 439 and name CA)	12.94	0.64	0.64
	assign (segid 3A4 and resid 272 and name CA)	(segid 3A4 and resid 440 and name CA)	11.64	0.86	0.87
	assign (segid 3A4 and resid 272 and name CB)	(segid 3A4 and resid 273 and name C)	5.80	0.08	0.08
80	assign (segid 3A4 and resid 272 and name CB)	(segid 3A4 and resid 273 and name CA)	4.62	0.05	0.06
	assign (segid 3A4 and resid 272 and name CB)	(segid 3A4 and resid 273 and name CB)	5.02	0.09	0.09
	assign (segid 3A4 and resid 272 and name CB)	(segid 3A4 and resid 273 and name N)	3.38	0.08	0.08
	assign (segid 3A4 and resid 272 and name CB)	(segid 3A4 and resid 273 and name O)	6.61	0.15	0.15

5	assign	(segid 3A4 and resid 272 and name CB)	(segid 3A4 and resid 274 and name CA)	7.55	0.09	0.10
	assign	(segid 3A4 and resid 272 and name CB)	(segid 3A4 and resid 274 and name CB)	8.02	0.11	0.10
	assign	(segid 3A4 and resid 272 and name CB)	(segid 3A4 and resid 274 and name N)	6.26	0.06	0.06
	assign	(segid 3A4 and resid 272 and name CB)	(segid 3A4 and resid 275 and name CA)	10.04	0.06	0.06
	assign	(segid 3A4 and resid 272 and name CB)	(segid 3A4 and resid 275 and name CB)	10.33	0.12	0.12
10	assign	(segid 3A4 and resid 272 and name CB)	(segid 3A4 and resid 276 and name CA)	9.67	0.11	0.11
	assign	(segid 3A4 and resid 272 and name CB)	(segid 3A4 and resid 276 and name CB)	8.72	0.16	0.15
	assign	(segid 3A4 and resid 272 and name CB)	(segid 3A4 and resid 277 and name CA)	10.08	0.32	0.32
	assign	(segid 3A4 and resid 272 and name CB)	(segid 3A4 and resid 277 and name CB)	9.39	0.43	0.43
	assign	(segid 3A4 and resid 272 and name CB)	(segid 3A4 and resid 278 and name CA)	12.98	0.20	0.21
15	assign	(segid 3A4 and resid 272 and name CB)	(segid 3A4 and resid 278 and name CB)	13.11	0.17	0.17
	assign	(segid 3A4 and resid 272 and name CB)	(segid 3A4 and resid 279 and name CA)	14.53	0.12	0.11
	assign	(segid 3A4 and resid 272 and name CB)	(segid 3A4 and resid 279 and name CB)	14.06	0.18	0.18
	assign	(segid 3A4 and resid 272 and name CB)	(segid 3A4 and resid 280 and name CA)	14.59	0.34	0.35
	assign	(segid 3A4 and resid 272 and name CB)	(segid 3A4 and resid 280 and name CB)	13.58	0.44	0.43
20	assign	(segid 3A4 and resid 272 and name CB)	(segid 3A4 and resid 281 and name CA)	16.10	0.49	0.49
	assign	(segid 3A4 and resid 272 and name CB)	(segid 3A4 and resid 281 and name CB)	15.59	0.49	0.49
	assign	(segid 3A4 and resid 272 and name CB)	(segid 3A4 and resid 282 and name CA)	18.58	0.35	0.36
	assign	(segid 3A4 and resid 272 and name CB)	(segid 3A4 and resid 304 and name CA)	18.06	0.64	0.64
	assign	(segid 3A4 and resid 272 and name CB)	(segid 3A4 and resid 304 and name CB)	17.38	0.53	0.53
25	assign	(segid 3A4 and resid 272 and name CB)	(segid 3A4 and resid 305 and name CA)	16.93	0.64	0.64
	assign	(segid 3A4 and resid 272 and name CB)	(segid 3A4 and resid 305 and name CB)	17.56	0.55	0.55
	assign	(segid 3A4 and resid 272 and name CB)	(segid 3A4 and resid 307 and name CA)	17.35	0.90	0.89
	assign	(segid 3A4 and resid 272 and name CB)	(segid 3A4 and resid 307 and name CB)	17.54	0.97	0.96
	assign	(segid 3A4 and resid 272 and name CB)	(segid 3A4 and resid 308 and name CA)	13.81	0.84	0.84
30	assign	(segid 3A4 and resid 272 and name CB)	(segid 3A4 and resid 308 and name CB)	13.34	0.85	0.85
	assign	(segid 3A4 and resid 272 and name CB)	(segid 3A4 and resid 309 and name CA)	15.19	0.79	0.78
	assign	(segid 3A4 and resid 272 and name CB)	(segid 3A4 and resid 309 and name CB)	16.46	0.82	0.81
	assign	(segid 3A4 and resid 272 and name CB)	(segid 3A4 and resid 310 and name CA)	16.85	0.73	0.73
	assign	(segid 3A4 and resid 272 and name CB)	(segid 3A4 and resid 310 and name CB)	17.89	0.79	0.78
35	assign	(segid 3A4 and resid 272 and name CB)	(segid 3A4 and resid 311 and name CA)	13.92	0.77	0.77
	assign	(segid 3A4 and resid 272 and name CB)	(segid 3A4 and resid 311 and name CB)	13.27	0.85	0.86
	assign	(segid 3A4 and resid 272 and name CB)	(segid 3A4 and resid 312 and name CA)	12.01	0.62	0.63
	assign	(segid 3A4 and resid 272 and name CB)	(segid 3A4 and resid 312 and name CB)	11.87	0.61	0.60
	assign	(segid 3A4 and resid 272 and name CB)	(segid 3A4 and resid 313 and name CA)	15.31	0.59	0.58
40	assign	(segid 3A4 and resid 272 and name CB)	(segid 3A4 and resid 313 and name CB)	16.63	0.59	0.59
	assign	(segid 3A4 and resid 272 and name CB)	(segid 3A4 and resid 314 and name CA)	15.66	0.56	0.57
	assign	(segid 3A4 and resid 272 and name CB)	(segid 3A4 and resid 314 and name CB)	15.85	0.64	0.63
	assign	(segid 3A4 and resid 272 and name CB)	(segid 3A4 and resid 315 and name CA)	12.48	0.54	0.53
	assign	(segid 3A4 and resid 272 and name CB)	(segid 3A4 and resid 315 and name CB)	11.16	0.55	0.55
45	assign	(segid 3A4 and resid 272 and name CB)	(segid 3A4 and resid 316 and name CA)	12.69	0.54	0.55
	assign	(segid 3A4 and resid 272 and name CB)	(segid 3A4 and resid 317 and name CA)	16.34	0.49	0.49
	assign	(segid 3A4 and resid 272 and name CB)	(segid 3A4 and resid 318 and name CA)	17.31	0.59	0.60
	assign	(segid 3A4 and resid 272 and name CB)	(segid 3A4 and resid 318 and name CB)	17.18	0.52	0.52
	assign	(segid 3A4 and resid 272 and name CB)	(segid 3A4 and resid 352 and name CA)	18.07	0.42	0.41
50	assign	(segid 3A4 and resid 272 and name CB)	(segid 3A4 and resid 352 and name CB)	17.44	0.49	0.49
	assign	(segid 3A4 and resid 272 and name CB)	(segid 3A4 and resid 359 and name CA)	16.46	0.80	0.81
	assign	(segid 3A4 and resid 272 and name CB)	(segid 3A4 and resid 359 and name CB)	15.98	0.87	0.87
	assign	(segid 3A4 and resid 272 and name CB)	(segid 3A4 and resid 360 and name CA)	15.67	0.58	0.58
	assign	(segid 3A4 and resid 272 and name CB)	(segid 3A4 and resid 360 and name CB)	16.82	0.52	0.52

	assign (segid 3A4 and resid 272 and name CB)	(segid 3A4 and resid 435 and name CA)	12.97	0.84	0.84
	assign (segid 3A4 and resid 272 and name CB)	(segid 3A4 and resid 436 and name CA)	15.27	1.57	1.57
	assign (segid 3A4 and resid 272 and name CB)	(segid 3A4 and resid 437 and name CA)	14.56	0.88	0.89
	assign (segid 3A4 and resid 272 and name CB)	(segid 3A4 and resid 438 and name CA)	11.80	0.64	0.64
5	assign (segid 3A4 and resid 272 and name CB)	(segid 3A4 and resid 439 and name CA)	13.04	0.67	0.66
	assign (segid 3A4 and resid 272 and name CB)	(segid 3A4 and resid 440 and name CA)	12.15	0.88	0.87
	assign (segid 3A4 and resid 272 and name N)	(segid 3A4 and resid 272 and name C)	2.47	0.04	0.04
	assign (segid 3A4 and resid 272 and name N)	(segid 3A4 and resid 272 and name CB)	1.45	0.01	0.01
	assign (segid 3A4 and resid 272 and name N)	(segid 3A4 and resid 272 and name O)	2.45	0.02	0.02
10	assign (segid 3A4 and resid 272 and name N)	(segid 3A4 and resid 273 and name C)	3.59	0.05	0.04
	assign (segid 3A4 and resid 272 and name N)	(segid 3A4 and resid 273 and name CB)	4.81	0.07	0.07
	assign (segid 3A4 and resid 272 and name N)	(segid 3A4 and resid 273 and name O)	4.19	0.03	0.03
	assign (segid 3A4 and resid 272 and name N)	(segid 3A4 and resid 273 and name N)	4.98	0.08	0.07
	assign (segid 3A4 and resid 272 and name N)	(segid 3A4 and resid 273 and name O)	2.76	0.03	0.03
15	assign (segid 3A4 and resid 272 and name N)	(segid 3A4 and resid 274 and name C)	5.53	0.09	0.08
	assign (segid 3A4 and resid 272 and name N)	(segid 3A4 and resid 274 and name CB)	7.35	0.13	0.12
	assign (segid 3A4 and resid 272 and name N)	(segid 3A4 and resid 274 and name O)	6.11	0.19	0.19
	assign (segid 3A4 and resid 272 and name N)	(segid 3A4 and resid 274 and name N)	6.62	0.28	0.29
	assign (segid 3A4 and resid 272 and name N)	(segid 3A4 and resid 274 and name CB)	5.09	0.15	0.14
20	assign (segid 3A4 and resid 272 and name N)	(segid 3A4 and resid 272 and name CB)	3.03	0.10	0.11
	assign (segid 3A4 and resid 272 and name O)	(segid 3A4 and resid 273 and name C)	3.95	0.03	0.04
	assign (segid 3A4 and resid 272 and name O)	(segid 3A4 and resid 273 and name CB)	2.75	0.02	0.02
	assign (segid 3A4 and resid 272 and name O)	(segid 3A4 and resid 273 and name O)	3.67	0.05	0.05
	assign (segid 3A4 and resid 272 and name O)	(segid 3A4 and resid 273 and name N)	2.23	0.01	0.01
25	assign (segid 3A4 and resid 272 and name O)	(segid 3A4 and resid 273 and name O)	5.06	0.03	0.03
	assign (segid 3A4 and resid 272 and name O)	(segid 3A4 and resid 274 and name C)	6.58	0.08	0.08
	assign (segid 3A4 and resid 272 and name O)	(segid 3A4 and resid 274 and name CB)	5.55	0.07	0.07
	assign (segid 3A4 and resid 272 and name O)	(segid 3A4 and resid 274 and name O)	5.82	0.11	0.10
	assign (segid 3A4 and resid 272 and name O)	(segid 3A4 and resid 274 and name N)	4.14	0.06	0.06
30	assign (segid 3A4 and resid 272 and name O)	(segid 3A4 and resid 274 and name O)	7.69	0.10	0.11
	assign (segid 3A4 and resid 272 and name O)	(segid 3A4 and resid 275 and name CA)	7.73	0.12	0.11
	assign (segid 3A4 and resid 272 and name O)	(segid 3A4 and resid 275 and name N)	6.48	0.07	0.07
	assign (segid 3A4 and resid 272 and name O)	(segid 3A4 and resid 276 and name CG2)	7.51	0.22	0.23
	assign (segid 3A4 and resid 272 and name O)	(segid 3A4 and resid 276 and name N)	7.52	0.14	0.14
35	assign (segid 3A4 and resid 272 and name O)	(segid 3A4 and resid 273 and name CB)	2.51	0.02	0.02
	assign (segid 3A4 and resid 273 and name C)	(segid 3A4 and resid 273 and name O)	1.23	0.00	0.01
	assign (segid 3A4 and resid 273 and name C)	(segid 3A4 and resid 274 and name C)	3.05	0.04	0.04
	assign (segid 3A4 and resid 273 and name C)	(segid 3A4 and resid 274 and name CA)	2.47	0.02	0.02
	assign (segid 3A4 and resid 273 and name C)	(segid 3A4 and resid 274 and name CB)	3.64	0.01	0.01
40	assign (segid 3A4 and resid 273 and name C)	(segid 3A4 and resid 274 and name N)	1.35	0.01	0.00
	assign (segid 3A4 and resid 273 and name C)	(segid 3A4 and resid 274 and name O)	4.02	0.10	0.11
	assign (segid 3A4 and resid 273 and name C)	(segid 3A4 and resid 275 and name C)	4.60	0.07	0.08
	assign (segid 3A4 and resid 273 and name C)	(segid 3A4 and resid 275 and name CA)	4.36	0.04	0.03
	assign (segid 3A4 and resid 273 and name C)	(segid 3A4 and resid 275 and name CB)	4.99	0.07	0.08
45	assign (segid 3A4 and resid 273 and name C)	(segid 3A4 and resid 275 and name N)	3.13	0.04	0.05
	assign (segid 3A4 and resid 273 and name C)	(segid 3A4 and resid 275 and name O)	5.77	0.10	0.09
	assign (segid 3A4 and resid 273 and name C)	(segid 3A4 and resid 276 and name C)	5.14	0.17	0.17
	assign (segid 3A4 and resid 273 and name C)	(segid 3A4 and resid 276 and name CA)	4.68	0.10	0.10
	assign (segid 3A4 and resid 273 and name C)	(segid 3A4 and resid 276 and name CB)	4.47	0.11	0.11
50	assign (segid 3A4 and resid 273 and name C)	(segid 3A4 and resid 276 and name CG2)	4.79	0.22	0.22
	assign (segid 3A4 and resid 273 and name C)	(segid 3A4 and resid 276 and name N)	3.84	0.09	0.09
	assign (segid 3A4 and resid 273 and name C)	(segid 3A4 and resid 277 and name C)	6.36	0.17	0.17
	assign (segid 3A4 and resid 273 and name C)	(segid 3A4 and resid 277 and name CA)	5.43	0.28	0.28
	assign (segid 3A4 and resid 273 and name C)	(segid 3A4 and resid 277 and name CB)	5.06	0.35	0.35
55	assign (segid 3A4 and resid 273 and name C)	(segid 3A4 and resid 277 and name N)	4.46	0.23	0.24
	assign (segid 3A4 and resid 273 and name C)	(segid 3A4 and resid 278 and name CA)	7.54	0.18	0.17
	assign (segid 3A4 and resid 273 and name C)	(segid 3A4 and resid 278 and name CB)	7.48	0.13	0.12
	assign (segid 3A4 and resid 273 and name C)	(segid 3A4 and resid 278 and name N)	6.30	0.20	0.21
60	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 273 and name C)	1.51	0.01	0.01
	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 273 and name CB)	1.54	0.02	0.01
	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 273 and name O)	2.40	0.01	0.02
	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 274 and name C)	4.48	0.05	0.05
	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 274 and name CA)	3.83	0.03	0.02
65	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 274 and name CB)	4.73	0.03	0.03
	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 274 and name N)	2.44	0.03	0.03
	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 274 and name O)	5.51	0.10	0.11
	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 275 and name C)	5.73	0.09	0.10
	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 275 and name CA)	5.48	0.06	0.05
70	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 275 and name CB)	5.78	0.10	0.10
	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 275 and name N)	4.34	0.04	0.03
	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 275 and name O)	6.92	0.11	0.11
	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 276 and name C)	6.22	0.22	0.22
	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 276 and name CA)	5.57	0.15	0.15
75	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 276 and name CB)	5.00	0.15	0.16
	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 276 and name CG2)	5.00	0.24	0.24
	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 276 and name N)	4.85	0.12	0.13
	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 276 and name O)	7.43	0.22	0.22
	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 277 and name CA)	6.70	0.32	0.33
80	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 277 and name CB)	6.36	0.40	0.40
	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 277 and name N)	5.69	0.28	0.28
	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 278 and name CA)	8.99	0.18	0.18
	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 278 and name CB)	8.94	0.12	0.11

	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 279 and name CA)	10.36	0.20	0.21
	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 279 and name CB)	9.85	0.30	0.29
	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 280 and name CA)	11.20	0.22	0.23
	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 280 and name CB)	10.51	0.28	0.29
	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 281 and name CA)	12.79	0.33	0.33
5	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 281 and name CB)	12.32	0.35	0.35
	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 282 and name CA)	14.72	0.23	0.23
	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 303 and name CA)	18.29	0.26	0.26
	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 303 and name CB)	19.12	0.32	0.32
10	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 304 and name CA)	14.96	0.46	0.45
	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 304 and name CB)	14.03	0.36	0.36
	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 305 and name CA)	14.56	0.48	0.48
	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 305 and name CB)	15.30	0.45	0.45
	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 306 and name CA)	16.95	0.54	0.53
	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 307 and name CA)	15.17	0.68	0.68
15	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 307 and name CB)	15.02	0.77	0.77
	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 308 and name CA)	11.94	0.58	0.57
	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 308 and name CB)	11.29	0.58	0.59
	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 309 and name CA)	14.31	0.52	0.53
	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 309 and name CB)	15.58	0.55	0.55
20	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 310 and name CA)	15.99	0.48	0.49
	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 310 and name CB)	16.74	0.56	0.56
	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 311 and name CA)	13.08	0.50	0.51
	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 311 and name CB)	12.03	0.58	0.57
	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 312 and name CA)	12.21	0.37	0.37
25	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 312 and name CB)	12.06	0.40	0.40
	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 313 and name CA)	15.92	0.38	0.38
	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 313 and name CB)	17.05	0.37	0.37
	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 314 and name CA)	16.08	0.37	0.38
	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 314 and name CB)	15.88	0.44	0.44
30	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 315 and name CA)	13.47	0.46	0.46
	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 315 and name CB)	11.97	0.46	0.47
	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 316 and name CA)	14.64	0.51	0.51
	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 317 and name CA)	18.16	0.39	0.39
	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 352 and name CA)	18.93	0.46	0.46
35	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 352 and name CB)	18.64	0.54	0.55
	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 357 and name CA)	18.36	0.51	0.52
	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 359 and name CA)	15.81	0.68	0.67
	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 359 and name CB)	15.01	0.71	0.70
	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 360 and name CA)	15.71	0.50	0.50
40	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 360 and name CB)	17.09	0.49	0.49
	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 361 and name CA)	13.41	0.50	0.51
	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 361 and name CB)	13.96	0.56	0.57
	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 362 and name CA)	10.54	0.61	0.62
	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 362 and name CB)	10.91	0.77	0.77
45	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 363 and name CA)	8.46	0.60	0.60
	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 363 and name CB)	7.36	0.59	0.59
	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 364 and name CA)	9.62	0.84	0.84
	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 364 and name CB)	10.58	0.89	0.90
	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 365 and name CA)	10.87	0.71	0.70
50	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 365 and name CB)	10.31	0.66	0.67
	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 401 and name CA)	18.15	0.48	0.49
	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 402 and name CA)	18.08	0.37	0.38
	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 402 and name CB)	19.00	0.32	0.33
	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 404 and name CA)	18.25	0.74	0.75
55	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 404 and name CB)	18.12	0.83	0.83
	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 405 and name CA)	14.85	0.61	0.61
	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 405 and name CB)	14.07	0.51	0.51
	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 406 and name CA)	16.56	0.68	0.67
	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 407 and name CA)	18.44	0.60	0.60
60	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 408 and name CA)	15.97	0.57	0.58
	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 408 and name CB)	15.14	0.61	0.61
	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 409 and name CA)	13.68	0.51	0.52
	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 409 and name CB)	12.73	0.50	0.50
	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 410 and name CA)	16.81	0.48	0.48
65	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 411 and name CA)	18.20	0.65	0.65
	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 411 and name CB)	18.90	0.58	0.58
	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 412 and name CA)	15.54	0.89	0.89
	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 413 and name CA)	12.61	1.46	1.45
	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 413 and name CB)	11.27	1.37	1.37
70	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 414 and name CA)	10.92	0.74	0.75
	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 415 and name CA)	11.41	0.94	0.95
	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 415 and name CB)	11.77	0.98	0.97
	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 416 and name CA)	14.74	0.48	0.48
	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 417 and name CA)	14.72	1.41	1.42
75	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 423 and name CA)	14.30	1.49	1.49
	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 424 and name CA)	16.26	1.62	1.63
	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 425 and name CA)	17.76	0.71	0.71
	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 426 and name CA)	18.47	0.54	0.55
	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 435 and name CA)	16.76	0.66	0.66
80	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 435 and name CB)	18.44	0.76	0.76
	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 437 and name CA)	15.36	0.55	0.55
	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 438 and name CA)	16.18	0.60	0.59
	assign (segid 3A4 and resid 273 and name CA)	(segid 3A4 and resid 439 and name CA)			

	assign (segid 3A4 and resid 273 and name CA) (segid 3A4 and resid 440 and name CA)	14.37	0.78	0.77
	assign (segid 3A4 and resid 273 and name CB) (segid 3A4 and resid 274 and name C)	5.27	0.04	0.03
	assign (segid 3A4 and resid 273 and name CB) (segid 3A4 and resid 274 and name CA)	4.96	0.03	0.03
	assign (segid 3A4 and resid 273 and name CB) (segid 3A4 and resid 274 and name CB)	6.04	0.02	0.01
5	assign (segid 3A4 and resid 273 and name CB) (segid 3A4 and resid 274 and name N)	3.73	0.01	0.01
	assign (segid 3A4 and resid 273 and name CB) (segid 3A4 and resid 274 and name O)	6.19	0.10	0.11
	assign (segid 3A4 and resid 273 and name CB) (segid 3A4 and resid 275 and name C)	5.71	0.11	0.11
	assign (segid 3A4 and resid 273 and name CB) (segid 3A4 and resid 275 and name CA)	5.75	0.08	0.08
	assign (segid 3A4 and resid 273 and name CB) (segid 3A4 and resid 275 and name CB)	5.88	0.12	0.12
10	assign (segid 3A4 and resid 273 and name CB) (segid 3A4 and resid 275 and name N)	4.91	0.07	0.07
	assign (segid 3A4 and resid 273 and name CB) (segid 3A4 and resid 275 and name O)	6.84	0.11	0.12
	assign (segid 3A4 and resid 273 and name CB) (segid 3A4 and resid 276 and name C)	5.95	0.25	0.24
	assign (segid 3A4 and resid 273 and name CB) (segid 3A4 and resid 276 and name CA)	5.08	0.18	0.18
	assign (segid 3A4 and resid 273 and name CB) (segid 3A4 and resid 276 and name CB)	4.19	0.20	0.20
15	assign (segid 3A4 and resid 273 and name CB) (segid 3A4 and resid 276 and name CG2)	3.92	0.25	0.24
	assign (segid 3A4 and resid 273 and name CB) (segid 3A4 and resid 276 and name N)	4.64	0.13	0.13
	assign (segid 3A4 and resid 273 and name CB) (segid 3A4 and resid 276 and name O)	7.07	0.26	0.26
	assign (segid 3A4 and resid 273 and name CB) (segid 3A4 and resid 277 and name CA)	6.87	0.34	0.34
	assign (segid 3A4 and resid 273 and name CB) (segid 3A4 and resid 277 and name CB)	6.83	0.40	0.40
20	assign (segid 3A4 and resid 273 and name CB) (segid 3A4 and resid 277 and name N)	5.70	0.30	0.31
	assign (segid 3A4 and resid 273 and name CB) (segid 3A4 and resid 278 and name CA)	9.32	0.18	0.18
	assign (segid 3A4 and resid 273 and name CB) (segid 3A4 and resid 278 and name CB)	9.37	0.12	0.11
	assign (segid 3A4 and resid 273 and name CB) (segid 3A4 and resid 279 and name CA)	10.13	0.23	0.22
	assign (segid 3A4 and resid 273 and name CB) (segid 3A4 and resid 279 and name CB)	9.43	0.32	0.32
25	assign (segid 3A4 and resid 273 and name CB) (segid 3A4 and resid 280 and name CA)	10.88	0.24	0.24
	assign (segid 3A4 and resid 273 and name CB) (segid 3A4 and resid 280 and name CB)	10.16	0.31	0.30
	assign (segid 3A4 and resid 273 and name CB) (segid 3A4 and resid 281 and name CA)	12.90	0.32	0.32
	assign (segid 3A4 and resid 273 and name CB) (segid 3A4 and resid 281 and name CB)	12.60	0.34	0.33
	assign (segid 3A4 and resid 273 and name CB) (segid 3A4 and resid 282 and name CA)	14.74	0.21	0.20
30	assign (segid 3A4 and resid 273 and name CB) (segid 3A4 and resid 303 and name CA)	17.52	0.33	0.32
	assign (segid 3A4 and resid 273 and name CB) (segid 3A4 and resid 303 and name CB)	18.33	0.41	0.41
	assign (segid 3A4 and resid 273 and name CB) (segid 3A4 and resid 304 and name CA)	14.09	0.49	0.48
	assign (segid 3A4 and resid 273 and name CB) (segid 3A4 and resid 304 and name CB)	13.21	0.36	0.37
	assign (segid 3A4 and resid 273 and name CB) (segid 3A4 and resid 305 and name CA)	13.77	0.49	0.50
35	assign (segid 3A4 and resid 273 and name CB) (segid 3A4 and resid 305 and name CB)	14.63	0.45	0.45
	assign (segid 3A4 and resid 273 and name CB) (segid 3A4 and resid 306 and name CA)	15.93	0.55	0.55
	assign (segid 3A4 and resid 273 and name CB) (segid 3A4 and resid 307 and name CA)	13.96	0.70	0.69
	assign (segid 3A4 and resid 273 and name CB) (segid 3A4 and resid 307 and name CB)	13.81	0.79	0.79
	assign (segid 3A4 and resid 273 and name CB) (segid 3A4 and resid 308 and name CA)	10.80	0.57	0.58
40	assign (segid 3A4 and resid 273 and name CB) (segid 3A4 and resid 308 and name CB)	10.30	0.59	0.59
	assign (segid 3A4 and resid 273 and name CB) (segid 3A4 and resid 309 and name CA)	13.25	0.53	0.52
	assign (segid 3A4 and resid 273 and name CB) (segid 3A4 and resid 309 and name CB)	14.58	0.55	0.54
	assign (segid 3A4 and resid 273 and name CB) (segid 3A4 and resid 310 and name CA)	14.70	0.49	0.48
	assign (segid 3A4 and resid 273 and name CB) (segid 3A4 and resid 310 and name CB)	15.41	0.56	0.56
45	assign (segid 3A4 and resid 273 and name CB) (segid 3A4 and resid 311 and name CA)	11.68	0.50	0.50
	assign (segid 3A4 and resid 273 and name CB) (segid 3A4 and resid 311 and name CB)	10.60	0.57	0.57
	assign (segid 3A4 and resid 273 and name CB) (segid 3A4 and resid 312 and name CA)	11.01	0.38	0.38
	assign (segid 3A4 and resid 273 and name CB) (segid 3A4 and resid 312 and name CB)	10.98	0.44	0.44
	assign (segid 3A4 and resid 273 and name CB) (segid 3A4 and resid 313 and name CA)	14.72	0.39	0.38
50	assign (segid 3A4 and resid 273 and name CB) (segid 3A4 and resid 313 and name CB)	15.84	0.38	0.38
	assign (segid 3A4 and resid 273 and name CB) (segid 3A4 and resid 314 and name CA)	14.71	0.37	0.37
	assign (segid 3A4 and resid 273 and name CB) (segid 3A4 and resid 314 and name CB)	14.45	0.42	0.43
	assign (segid 3A4 and resid 273 and name CB) (segid 3A4 and resid 315 and name CA)	12.17	0.45	0.45
	assign (segid 3A4 and resid 273 and name CB) (segid 3A4 and resid 315 and name CB)	10.67	0.46	0.46
55	assign (segid 3A4 and resid 273 and name CB) (segid 3A4 and resid 316 and name CA)	13.58	0.52	0.52
	assign (segid 3A4 and resid 273 and name CB) (segid 3A4 and resid 317 and name CA)	17.04	0.40	0.41
	assign (segid 3A4 and resid 273 and name CB) (segid 3A4 and resid 318 and name CA)	18.75	0.40	0.41
	assign (segid 3A4 and resid 273 and name CB) (segid 3A4 and resid 318 and name CB)	18.59	0.35	0.34
60	assign (segid 3A4 and resid 273 and name CB) (segid 3A4 and resid 351 and name CA)	18.43	0.42	0.42
	assign (segid 3A4 and resid 273 and name CB) (segid 3A4 and resid 352 and name CA)	17.58	0.44	0.43
	assign (segid 3A4 and resid 273 and name CB) (segid 3A4 and resid 352 and name CB)	17.35	0.52	0.52
	assign (segid 3A4 and resid 273 and name CB) (segid 3A4 and resid 357 and name CA)	17.82	0.58	0.57
	assign (segid 3A4 and resid 273 and name CB) (segid 3A4 and resid 357 and name CB)	16.87	0.49	0.49
65	assign (segid 3A4 and resid 273 and name CB) (segid 3A4 and resid 358 and name CA)	17.30	0.65	0.65
	assign (segid 3A4 and resid 273 and name CB) (segid 3A4 and resid 358 and name CB)	17.62	0.79	0.79
	assign (segid 3A4 and resid 273 and name CB) (segid 3A4 and resid 359 and name CA)	14.51	0.62	0.62
	assign (segid 3A4 and resid 273 and name CB) (segid 3A4 and resid 359 and name CB)	13.74	0.67	0.66
	assign (segid 3A4 and resid 273 and name CB) (segid 3A4 and resid 360 and name CA)	14.33	0.45	0.46
	assign (segid 3A4 and resid 273 and name CB) (segid 3A4 and resid 360 and name CB)	15.72	0.44	0.45
70	assign (segid 3A4 and resid 273 and name CB) (segid 3A4 and resid 361 and name CA)	12.21	0.47	0.46
	assign (segid 3A4 and resid 273 and name CB) (segid 3A4 and resid 361 and name CB)	12.85	0.52	0.52
	assign (segid 3A4 and resid 273 and name CB) (segid 3A4 and resid 362 and name CA)	9.25	0.56	0.57
	assign (segid 3A4 and resid 273 and name CB) (segid 3A4 and resid 362 and name CB)	9.63	0.73	0.73
	assign (segid 3A4 and resid 273 and name CB) (segid 3A4 and resid 363 and name CA)	6.99	0.57	0.57
75	assign (segid 3A4 and resid 273 and name CB) (segid 3A4 and resid 363 and name CB)	5.94	0.55	0.54
	assign (segid 3A4 and resid 273 and name CB) (segid 3A4 and resid 363 and name CG)	5.91	0.59	0.59
	assign (segid 3A4 and resid 273 and name CB) (segid 3A4 and resid 363 and name O)	5.95	0.77	0.77
	assign (segid 3A4 and resid 273 and name CB) (segid 3A4 and resid 364 and name CA)	8.14	0.85	0.86
	assign (segid 3A4 and resid 273 and name CB) (segid 3A4 and resid 364 and name CB)	9.14	0.91	0.91
80	assign (segid 3A4 and resid 273 and name CB) (segid 3A4 and resid 365 and name CA)	9.51	0.71	0.72
	assign (segid 3A4 and resid 273 and name CB) (segid 3A4 and resid 365 and name CB)	9.07	0.66	0.67
	assign (segid 3A4 and resid 273 and name CB) (segid 3A4 and resid 401 and name CA)	17.51	0.52	0.51
	assign (segid 3A4 and resid 273 and name CB) (segid 3A4 and resid 402 and name CA)	17.43	0.39	0.39

	assign (segid 3A4 and resid 273 and name CB)	(segid 3A4 and resid 402 and name CB)	18.28	0.33	0.33
	assign (segid 3A4 and resid 273 and name CB)	(segid 3A4 and resid 404 and name CA)	18.01	0.76	0.76
	assign (segid 3A4 and resid 273 and name CB)	(segid 3A4 and resid 404 and name CB)	17.84	0.85	0.85
	assign (segid 3A4 and resid 273 and name CB)	(segid 3A4 and resid 405 and name CA)	14.58	0.63	0.62
	assign (segid 3A4 and resid 273 and name CB)	(segid 3A4 and resid 405 and name CB)	13.67	0.54	0.55
5	assign (segid 3A4 and resid 273 and name CB)	(segid 3A4 and resid 406 and name CA)	16.34	0.65	0.65
	assign (segid 3A4 and resid 273 and name CB)	(segid 3A4 and resid 407 and name CA)	18.46	0.57	0.58
	assign (segid 3A4 and resid 273 and name CB)	(segid 3A4 and resid 408 and name CA)	16.20	0.56	0.56
	assign (segid 3A4 and resid 273 and name CB)	(segid 3A4 and resid 408 and name CB)	15.33	0.61	0.62
	assign (segid 3A4 and resid 273 and name CB)	(segid 3A4 and resid 409 and name CA)	13.98	0.50	0.50
10	assign (segid 3A4 and resid 273 and name CB)	(segid 3A4 and resid 409 and name CB)	12.93	0.47	0.47
	assign (segid 3A4 and resid 273 and name CB)	(segid 3A4 and resid 410 and name CA)	17.14	0.46	0.45
	assign (segid 3A4 and resid 273 and name CB)	(segid 3A4 and resid 412 and name CA)	16.28	0.85	0.85
	assign (segid 3A4 and resid 273 and name CB)	(segid 3A4 and resid 413 and name CA)	13.67	1.41	1.41
	assign (segid 3A4 and resid 273 and name CB)	(segid 3A4 and resid 414 and name CA)	12.30	1.30	1.30
15	assign (segid 3A4 and resid 273 and name CB)	(segid 3A4 and resid 415 and name CA)	12.08	0.76	0.77
	assign (segid 3A4 and resid 273 and name CB)	(segid 3A4 and resid 415 and name CB)	12.62	1.03	1.03
	assign (segid 3A4 and resid 273 and name CB)	(segid 3A4 and resid 416 and name CA)	12.86	0.94	0.94
	assign (segid 3A4 and resid 273 and name CB)	(segid 3A4 and resid 417 and name CA)	15.91	0.44	0.43
	assign (segid 3A4 and resid 273 and name CB)	(segid 3A4 and resid 423 and name CA)	15.31	1.47	1.48
20	assign (segid 3A4 and resid 273 and name CB)	(segid 3A4 and resid 424 and name CA)	14.61	1.61	1.61
	assign (segid 3A4 and resid 273 and name CB)	(segid 3A4 and resid 425 and name CA)	16.33	1.75	1.76
	assign (segid 3A4 and resid 273 and name CB)	(segid 3A4 and resid 426 and name CA)	17.60	0.76	0.76
	assign (segid 3A4 and resid 273 and name CB)	(segid 3A4 and resid 434 and name CA)	18.02	0.50	0.50
	assign (segid 3A4 and resid 273 and name CB)	(segid 3A4 and resid 435 and name CA)	16.57	0.63	0.64
25	assign (segid 3A4 and resid 273 and name CB)	(segid 3A4 and resid 437 and name CA)	18.73	0.71	0.72
	assign (segid 3A4 and resid 273 and name CB)	(segid 3A4 and resid 438 and name CA)	15.80	0.53	0.54
	assign (segid 3A4 and resid 273 and name CB)	(segid 3A4 and resid 439 and name CA)	16.93	0.61	0.60
	assign (segid 3A4 and resid 273 and name CB)	(segid 3A4 and resid 440 and name CA)	15.27	0.78	0.79
	assign (segid 3A4 and resid 273 and name CB)	(segid 3A4 and resid 273 and name C)	2.43	0.01	0.01
30	assign (segid 3A4 and resid 273 and name N)	(segid 3A4 and resid 273 and name CB)	1.45	0.01	0.01
	assign (segid 3A4 and resid 273 and name N)	(segid 3A4 and resid 273 and name O)	2.44	0.01	0.01
	assign (segid 3A4 and resid 273 and name N)	(segid 3A4 and resid 274 and name C)	3.30	0.04	0.04
	assign (segid 3A4 and resid 273 and name N)	(segid 3A4 and resid 274 and name CA)	5.37	0.04	0.05
	assign (segid 3A4 and resid 273 and name N)	(segid 3A4 and resid 274 and name CB)	4.40	0.03	0.04
35	assign (segid 3A4 and resid 273 and name N)	(segid 3A4 and resid 274 and name N)	5.18	0.06	0.05
	assign (segid 3A4 and resid 273 and name N)	(segid 3A4 and resid 274 and name O)	3.07	0.03	0.02
	assign (segid 3A4 and resid 273 and name N)	(segid 3A4 and resid 275 and name C)	6.32	0.10	0.10
	assign (segid 3A4 and resid 273 and name N)	(segid 3A4 and resid 275 and name CB)	6.94	0.08	0.09
	assign (segid 3A4 and resid 273 and name N)	(segid 3A4 and resid 275 and name CA)	6.73	0.05	0.05
40	assign (segid 3A4 and resid 273 and name N)	(segid 3A4 and resid 275 and name N)	7.16	0.09	0.10
	assign (segid 3A4 and resid 273 and name N)	(segid 3A4 and resid 276 and name C)	5.50	0.04	0.03
	assign (segid 3A4 and resid 273 and name N)	(segid 3A4 and resid 276 and name CA)	7.03	0.21	0.21
	assign (segid 3A4 and resid 273 and name N)	(segid 3A4 and resid 276 and name CB)	6.59	0.13	0.14
	assign (segid 3A4 and resid 273 and name N)	(segid 3A4 and resid 276 and name CG2)	5.91	0.14	0.14
45	assign (segid 3A4 and resid 273 and name N)	(segid 3A4 and resid 276 and name N)	6.07	0.25	0.24
	assign (segid 3A4 and resid 273 and name N)	(segid 3A4 and resid 277 and name CA)	6.02	0.10	0.11
	assign (segid 3A4 and resid 273 and name N)	(segid 3A4 and resid 277 and name CB)	7.14	0.34	0.34
	assign (segid 3A4 and resid 273 and name N)	(segid 3A4 and resid 277 and name N)	6.57	0.43	0.42
	assign (segid 3A4 and resid 273 and name N)	(segid 3A4 and resid 277 and name O)	6.34	0.27	0.27
50	assign (segid 3A4 and resid 273 and name O)	(segid 3A4 and resid 273 and name CB)	2.75	0.05	0.05
	assign (segid 3A4 and resid 273 and name O)	(segid 3A4 and resid 274 and name C)	2.85	0.06	0.07
	assign (segid 3A4 and resid 273 and name O)	(segid 3A4 and resid 274 and name CA)	2.79	0.05	0.04
	assign (segid 3A4 and resid 273 and name O)	(segid 3A4 and resid 274 and name CB)	4.21	0.03	0.03
	assign (segid 3A4 and resid 273 and name O)	(segid 3A4 and resid 274 and name N)	2.24	0.02	0.02
55	assign (segid 3A4 and resid 273 and name O)	(segid 3A4 and resid 274 and name O)	3.57	0.15	0.15
	assign (segid 3A4 and resid 273 and name O)	(segid 3A4 and resid 275 and name C)	3.79	0.09	0.08
	assign (segid 3A4 and resid 273 and name O)	(segid 3A4 and resid 275 and name CA)	3.92	0.07	0.07
	assign (segid 3A4 and resid 273 and name O)	(segid 3A4 and resid 275 and name CB)	4.72	0.09	0.08
	assign (segid 3A4 and resid 273 and name O)	(segid 3A4 and resid 275 and name N)	2.96	0.09	0.09
60	assign (segid 3A4 and resid 273 and name O)	(segid 3A4 and resid 275 and name O)	4.88	0.11	0.11
	assign (segid 3A4 and resid 273 and name O)	(segid 3A4 and resid 276 and name C)	3.93	0.18	0.19
	assign (segid 3A4 and resid 273 and name O)	(segid 3A4 and resid 276 and name CA)	3.52	0.10	0.10
	assign (segid 3A4 and resid 273 and name O)	(segid 3A4 and resid 276 and name CB)	3.37	0.11	0.11
	assign (segid 3A4 and resid 273 and name O)	(segid 3A4 and resid 276 and name CG2)	3.92	0.23	0.24
65	assign (segid 3A4 and resid 273 and name O)	(segid 3A4 and resid 276 and name N)	2.85	0.09	0.09
	assign (segid 3A4 and resid 273 and name O)	(segid 3A4 and resid 276 and name O)	5.16	0.19	0.19
	assign (segid 3A4 and resid 273 and name O)	(segid 3A4 and resid 277 and name C)	5.52	0.28	0.29
	assign (segid 3A4 and resid 273 and name O)	(segid 3A4 and resid 277 and name CA)	4.43	0.31	0.31
	assign (segid 3A4 and resid 273 and name O)	(segid 3A4 and resid 277 and name CB)	4.32	0.36	0.37
70	assign (segid 3A4 and resid 273 and name O)	(segid 3A4 and resid 277 and name N)	3.34	0.27	0.27
	assign (segid 3A4 and resid 273 and name O)	(segid 3A4 and resid 277 and name O)	6.68	0.28	0.29
	assign (segid 3A4 and resid 273 and name O)	(segid 3A4 and resid 278 and name C)	7.50	0.21	0.21
	assign (segid 3A4 and resid 273 and name O)	(segid 3A4 and resid 278 and name CA)	6.70	0.22	0.22
	assign (segid 3A4 and resid 273 and name O)	(segid 3A4 and resid 278 and name CB)	6.79	0.16	0.17
75	assign (segid 3A4 and resid 273 and name O)	(segid 3A4 and resid 278 and name N)	5.41	0.24	0.23
	assign (segid 3A4 and resid 273 and name O)	(segid 3A4 and resid 279 and name N)	7.05	0.20	0.20
	assign (segid 3A4 and resid 273 and name O)	(segid 3A4 and resid 274 and name CB)	2.53	0.02	0.02
	assign (segid 3A4 and resid 274 and name C)	(segid 3A4 and resid 274 and name O)	1.24	0.02	0.01
80	assign (segid 3A4 and resid 274 and name C)	(segid 3A4 and resid 275 and name C)	3.03	0.04	0.05
	assign (segid 3A4 and resid 274 and name C)	(segid 3A4 and resid 275 and name CA)	2.43	0.02	0.02
	assign (segid 3A4 and resid 274 and name C)	(segid 3A4 and resid 275 and name CB)	3.70	0.04	0.04
	assign (segid 3A4 and resid 274 and name C)	(segid 3A4 and resid 275 and name N)	1.33	0.00	0.01

	assign (segid 3A4 and resid 274 and name C)	(segid 3A4 and resid 275 and name O)	3.95	0.08	0.07
	assign (segid 3A4 and resid 274 and name C)	(segid 3A4 and resid 276 and name C)	1.49	0.06	0.06
	assign (segid 3A4 and resid 274 and name C)	(segid 3A4 and resid 276 and name CA)	4.40	0.06	0.06
	assign (segid 3A4 and resid 274 and name C)	(segid 3A4 and resid 276 and name CB)	5.16	0.11	0.11
5	assign (segid 3A4 and resid 274 and name C)	(segid 3A4 and resid 276 and name CG2)	5.76	0.18	0.17
	assign (segid 3A4 and resid 274 and name C)	(segid 3A4 and resid 276 and name N)	3.20	0.04	0.05
	assign (segid 3A4 and resid 274 and name C)	(segid 3A4 and resid 276 and name O)	5.56	0.08	0.09
	assign (segid 3A4 and resid 274 and name C)	(segid 3A4 and resid 277 and name C)	4.89	0.10	0.09
	assign (segid 3A4 and resid 274 and name C)	(segid 3A4 and resid 277 and name CA)	4.50	0.08	0.07
	assign (segid 3A4 and resid 274 and name C)	(segid 3A4 and resid 277 and name CB)	4.25	0.08	0.07
10	assign (segid 3A4 and resid 274 and name C)	(segid 3A4 and resid 277 and name N)	3.77	0.05	0.05
	assign (segid 3A4 and resid 274 and name C)	(segid 3A4 and resid 277 and name O)	6.10	0.09	0.10
	assign (segid 3A4 and resid 274 and name C)	(segid 3A4 and resid 278 and name C)	6.18	0.07	0.07
	assign (segid 3A4 and resid 274 and name C)	(segid 3A4 and resid 278 and name CA)	5.08	0.10	0.09
	assign (segid 3A4 and resid 274 and name C)	(segid 3A4 and resid 278 and name CB)	4.68	0.09	0.09
15	assign (segid 3A4 and resid 274 and name C)	(segid 3A4 and resid 278 and name N)	4.17	0.10	0.10
	assign (segid 3A4 and resid 274 and name C)	(segid 3A4 and resid 278 and name O)	7.34	0.07	0.07
	assign (segid 3A4 and resid 274 and name C)	(segid 3A4 and resid 279 and name CA)	7.32	0.08	0.09
	assign (segid 3A4 and resid 274 and name C)	(segid 3A4 and resid 279 and name CB)	7.28	0.14	0.15
	assign (segid 3A4 and resid 274 and name C)	(segid 3A4 and resid 279 and name N)	6.05	0.08	0.07
20	assign (segid 3A4 and resid 274 and name C)	(segid 3A4 and resid 280 and name N)	7.86	0.07	0.07
	assign (segid 3A4 and resid 274 and name C)	(segid 3A4 and resid 274 and name C)	1.51	0.01	0.02
	assign (segid 3A4 and resid 274 and name CA)	(segid 3A4 and resid 274 and name CB)	1.52	0.01	0.02
	assign (segid 3A4 and resid 274 and name CA)	(segid 3A4 and resid 274 and name O)	2.39	0.01	0.01
	assign (segid 3A4 and resid 274 and name CA)	(segid 3A4 and resid 275 and name C)	4.42	0.04	0.04
25	assign (segid 3A4 and resid 274 and name CA)	(segid 3A4 and resid 275 and name CA)	3.80	0.01	0.01
	assign (segid 3A4 and resid 274 and name CA)	(segid 3A4 and resid 275 and name CB)	4.87	0.03	0.03
	assign (segid 3A4 and resid 274 and name CA)	(segid 3A4 and resid 275 and name N)	2.44	0.02	0.03
	assign (segid 3A4 and resid 274 and name CA)	(segid 3A4 and resid 275 and name O)	5.40	0.07	0.07
	assign (segid 3A4 and resid 274 and name CA)	(segid 3A4 and resid 276 and name C)	5.40	0.08	0.08
30	assign (segid 3A4 and resid 274 and name CA)	(segid 3A4 and resid 276 and name CA)	5.37	0.09	0.10
	assign (segid 3A4 and resid 274 and name CA)	(segid 3A4 and resid 276 and name CB)	5.80	0.18	0.17
	assign (segid 3A4 and resid 274 and name CA)	(segid 3A4 and resid 276 and name CG2)	6.40	0.23	0.23
	assign (segid 3A4 and resid 274 and name CA)	(segid 3A4 and resid 276 and name N)	4.29	0.06	0.06
	assign (segid 3A4 and resid 274 and name CA)	(segid 3A4 and resid 276 and name O)	6.52	0.10	0.10
35	assign (segid 3A4 and resid 274 and name CA)	(segid 3A4 and resid 277 and name C)	5.66	0.11	0.11
	assign (segid 3A4 and resid 274 and name CA)	(segid 3A4 and resid 277 and name CA)	5.01	0.08	0.09
	assign (segid 3A4 and resid 274 and name CA)	(segid 3A4 and resid 277 and name CB)	4.34	0.11	0.11
	assign (segid 3A4 and resid 274 and name CA)	(segid 3A4 and resid 277 and name N)	4.46	0.08	0.07
	assign (segid 3A4 and resid 274 and name CA)	(segid 3A4 and resid 277 and name O)	6.84	0.12	0.13
40	assign (segid 3A4 and resid 274 and name CA)	(segid 3A4 and resid 278 and name C)	7.39	0.07	0.08
	assign (segid 3A4 and resid 274 and name CA)	(segid 3A4 and resid 278 and name CA)	6.18	0.10	0.10
	assign (segid 3A4 and resid 274 and name CA)	(segid 3A4 and resid 278 and name CB)	5.90	0.10	0.09
	assign (segid 3A4 and resid 274 and name CA)	(segid 3A4 and resid 278 and name N)	5.17	0.10	0.10
	assign (segid 3A4 and resid 274 and name CA)	(segid 3A4 and resid 279 and name CA)	8.65	0.07	0.08
45	assign (segid 3A4 and resid 274 and name CA)	(segid 3A4 and resid 279 and name CB)	8.64	0.16	0.15
	assign (segid 3A4 and resid 274 and name CA)	(segid 3A4 and resid 279 and name N)	7.35	0.06	0.07
	assign (segid 3A4 and resid 274 and name CA)	(segid 3A4 and resid 280 and name CA)	9.88	0.13	0.13
	assign (segid 3A4 and resid 274 and name CA)	(segid 3A4 and resid 280 and name CB)	9.48	0.24	0.24
	assign (segid 3A4 and resid 274 and name CA)	(segid 3A4 and resid 281 and name CA)	10.46	0.15	0.16
50	assign (segid 3A4 and resid 274 and name CA)	(segid 3A4 and resid 281 and name CB)	9.66	0.17	0.17
	assign (segid 3A4 and resid 274 and name CA)	(segid 3A4 and resid 282 and name CA)	12.26	0.16	0.16
	assign (segid 3A4 and resid 274 and name CA)	(segid 3A4 and resid 303 and name CA)	17.75	0.25	0.25
	assign (segid 3A4 and resid 274 and name CA)	(segid 3A4 and resid 303 and name CB)	18.53	0.22	0.21
	assign (segid 3A4 and resid 274 and name CA)	(segid 3A4 and resid 304 and name CA)	14.76	0.42	0.42
55	assign (segid 3A4 and resid 274 and name CA)	(segid 3A4 and resid 304 and name CB)	13.66	0.37	0.37
	assign (segid 3A4 and resid 274 and name CA)	(segid 3A4 and resid 305 and name CA)	14.52	0.57	0.56
	assign (segid 3A4 and resid 274 and name CA)	(segid 3A4 and resid 305 and name CB)	15.03	0.54	0.54
	assign (segid 3A4 and resid 274 and name CA)	(segid 3A4 and resid 306 and name CA)	17.54	0.60	0.59
	assign (segid 3A4 and resid 274 and name CA)	(segid 3A4 and resid 307 and name CA)	16.21	0.65	0.65
60	assign (segid 3A4 and resid 274 and name CA)	(segid 3A4 and resid 307 and name CB)	15.92	0.73	0.73
	assign (segid 3A4 and resid 274 and name CA)	(segid 3A4 and resid 308 and name CA)	13.11	0.56	0.56
	assign (segid 3A4 and resid 274 and name CA)	(segid 3A4 and resid 308 and name CB)	12.12	0.60	0.59
	assign (segid 3A4 and resid 274 and name CA)	(segid 3A4 and resid 309 and name CA)	15.72	0.61	0.61
	assign (segid 3A4 and resid 274 and name CA)	(segid 3A4 and resid 309 and name CB)	16.77	0.65	0.66
65	assign (segid 3A4 and resid 274 and name CA)	(segid 3A4 and resid 310 and name CA)	17.88	0.53	0.54
	assign (segid 3A4 and resid 274 and name CA)	(segid 3A4 and resid 310 and name CB)	18.54	0.59	0.59
	assign (segid 3A4 and resid 274 and name CA)	(segid 3A4 and resid 311 and name CA)	15.44	0.46	0.46
	assign (segid 3A4 and resid 274 and name CA)	(segid 3A4 and resid 311 and name CB)	14.29	0.49	0.50
	assign (segid 3A4 and resid 274 and name CA)	(segid 3A4 and resid 312 and name CA)	14.67	0.42	0.42
70	assign (segid 3A4 and resid 274 and name CA)	(segid 3A4 and resid 312 and name CB)	14.26	0.44	0.43
	assign (segid 3A4 and resid 274 and name CA)	(segid 3A4 and resid 313 and name CA)	18.46	0.43	0.44
	assign (segid 3A4 and resid 274 and name CA)	(segid 3A4 and resid 313 and name CB)	19.42	0.43	0.43
	assign (segid 3A4 and resid 274 and name CA)	(segid 3A4 and resid 314 and name CA)	19.01	0.35	0.36
	assign (segid 3A4 and resid 274 and name CA)	(segid 3A4 and resid 314 and name CB)	18.76	0.38	0.38
75	assign (segid 3A4 and resid 274 and name CA)	(segid 3A4 and resid 315 and name CA)	16.75	0.48	0.48
	assign (segid 3A4 and resid 274 and name CA)	(segid 3A4 and resid 315 and name CB)	15.25	0.49	0.50
	assign (segid 3A4 and resid 274 and name CA)	(segid 3A4 and resid 316 and name CA)	17.81	0.58	0.57
	assign (segid 3A4 and resid 274 and name CA)	(segid 3A4 and resid 359 and name CB)	18.02	0.60	0.59
	assign (segid 3A4 and resid 274 and name CA)	(segid 3A4 and resid 360 and name CA)	19.10	0.41	0.42
80	assign (segid 3A4 and resid 274 and name CA)	(segid 3A4 and resid 361 and name CA)	17.04	0.49	0.49
	assign (segid 3A4 and resid 274 and name CA)	(segid 3A4 and resid 361 and name CB)	17.63	0.56	0.57
	assign (segid 3A4 and resid 274 and name CA)	(segid 3A4 and resid 362 and name CA)	13.94	0.53	0.52

	assign (segid 3A4 and resid 274 and name CA) (segid 3A4 and resid 362 and name CB)	14.11	0.65	0.65
	assign (segid 3A4 and resid 274 and name CA) (segid 3A4 and resid 363 and name CA)	11.67	0.43	0.43
	assign (segid 3A4 and resid 274 and name CA) (segid 3A4 and resid 363 and name CB)	10.66	0.42	0.42
	assign (segid 3A4 and resid 274 and name CA) (segid 3A4 and resid 364 and name CA)	11.97	0.65	0.65
	assign (segid 3A4 and resid 274 and name CA) (segid 3A4 and resid 364 and name CB)	12.94	0.71	0.70
5	assign (segid 3A4 and resid 274 and name CA) (segid 3A4 and resid 365 and name CA)	12.42	0.61	0.60
	assign (segid 3A4 and resid 274 and name CA) (segid 3A4 and resid 365 and name CB)	11.50	0.62	0.62
	assign (segid 3A4 and resid 274 and name CA) (segid 3A4 and resid 401 and name CA)	18.90	0.45	0.44
	assign (segid 3A4 and resid 274 and name CA) (segid 3A4 and resid 402 and name CA)	18.30	0.35	0.35
	assign (segid 3A4 and resid 274 and name CA) (segid 3A4 and resid 402 and name CB)	19.24	0.33	0.32
10	assign (segid 3A4 and resid 274 and name CA) (segid 3A4 and resid 404 and name CA)	18.05	0.57	0.56
	assign (segid 3A4 and resid 274 and name CA) (segid 3A4 and resid 404 and name CB)	18.18	0.67	0.66
	assign (segid 3A4 and resid 274 and name CA) (segid 3A4 and resid 405 and name CA)	14.56	0.45	0.45
	assign (segid 3A4 and resid 274 and name CA) (segid 3A4 and resid 405 and name CB)	14.05	0.36	0.35
	assign (segid 3A4 and resid 274 and name CA) (segid 3A4 and resid 406 and name CA)	15.59	0.63	0.63
15	assign (segid 3A4 and resid 274 and name CA) (segid 3A4 and resid 407 and name CA)	17.15	0.49	0.49
	assign (segid 3A4 and resid 274 and name CA) (segid 3A4 and resid 407 and name CB)	18.47	0.42	0.42
	assign (segid 3A4 and resid 274 and name CA) (segid 3A4 and resid 408 and name CA)	14.73	0.42	0.42
	assign (segid 3A4 and resid 274 and name CA) (segid 3A4 and resid 408 and name CB)	14.20	0.40	0.40
20	assign (segid 3A4 and resid 274 and name CA) (segid 3A4 and resid 409 and name CA)	11.88	0.43	0.43
	assign (segid 3A4 and resid 274 and name CA) (segid 3A4 and resid 409 and name CB)	11.04	0.41	0.41
	assign (segid 3A4 and resid 274 and name CA) (segid 3A4 and resid 410 and name CA)	14.56	0.48	0.48
	assign (segid 3A4 and resid 274 and name CA) (segid 3A4 and resid 411 and name CA)	15.92	0.75	0.76
	assign (segid 3A4 and resid 274 and name CA) (segid 3A4 and resid 411 and name CB)	16.84	0.68	0.69
25	assign (segid 3A4 and resid 274 and name CA) (segid 3A4 and resid 412 and name CA)	13.20	1.00	0.99
	assign (segid 3A4 and resid 274 and name CA) (segid 3A4 and resid 413 and name CA)	10.04	1.25	1.24
	assign (segid 3A4 and resid 274 and name CA) (segid 3A4 and resid 414 and name CA)	9.66	1.14	1.14
	assign (segid 3A4 and resid 274 and name CA) (segid 3A4 and resid 415 and name CA)	9.96	0.91	0.90
	assign (segid 3A4 and resid 274 and name CA) (segid 3A4 and resid 415 and name CB)	10.32	0.90	0.91
30	assign (segid 3A4 and resid 274 and name CA) (segid 3A4 and resid 416 and name CA)	11.71	1.28	1.28
	assign (segid 3A4 and resid 274 and name CA) (segid 3A4 and resid 417 and name CA)	14.57	0.75	0.75
	assign (segid 3A4 and resid 274 and name CA) (segid 3A4 and resid 423 and name CA)	16.63	1.25	1.25
	assign (segid 3A4 and resid 274 and name CA) (segid 3A4 and resid 424 and name CA)	16.58	1.32	1.32
	assign (segid 3A4 and resid 274 and name CA) (segid 3A4 and resid 438 and name CA)	16.61	0.59	0.58
35	assign (segid 3A4 and resid 274 and name CA) (segid 3A4 and resid 439 and name CA)	16.65	0.57	0.57
	assign (segid 3A4 and resid 274 and name CA) (segid 3A4 and resid 440 and name CA)	14.10	0.65	0.64
	assign (segid 3A4 and resid 274 and name CB) (segid 3A4 and resid 275 and name C)	5.49	0.07	0.06
	assign (segid 3A4 and resid 274 and name CB) (segid 3A4 and resid 275 and name CA)	4.55	0.11	0.11
	assign (segid 3A4 and resid 274 and name CB) (segid 3A4 and resid 275 and name CB)	5.45	0.17	0.18
40	assign (segid 3A4 and resid 274 and name CB) (segid 3A4 and resid 275 and name N)	3.26	0.14	0.13
	assign (segid 3A4 and resid 274 and name CB) (segid 3A4 and resid 276 and name O)	6.40	0.08	0.09
	assign (segid 3A4 and resid 274 and name CB) (segid 3A4 and resid 276 and name CA)	6.80	0.11	0.11
	assign (segid 3A4 and resid 274 and name CB) (segid 3A4 and resid 276 and name CB)	6.76	0.08	0.08
	assign (segid 3A4 and resid 274 and name CB) (segid 3A4 and resid 276 and name N)	7.25	0.15	0.14
45	assign (segid 3A4 and resid 274 and name CB) (segid 3A4 and resid 277 and name C)	5.58	0.05	0.04
	assign (segid 3A4 and resid 274 and name CB) (segid 3A4 and resid 277 and name CA)	6.75	0.17	0.17
	assign (segid 3A4 and resid 274 and name CB) (segid 3A4 and resid 277 and name CB)	6.27	0.15	0.16
	assign (segid 3A4 and resid 274 and name CB) (segid 3A4 and resid 277 and name N)	5.46	0.19	0.19
50	assign (segid 3A4 and resid 274 and name CB) (segid 3A4 and resid 278 and name CA)	5.84	0.12	0.13
	assign (segid 3A4 and resid 274 and name CB) (segid 3A4 and resid 278 and name CB)	6.93	0.12	0.12
	assign (segid 3A4 and resid 274 and name CB) (segid 3A4 and resid 278 and name N)	6.41	0.10	0.10
	assign (segid 3A4 and resid 274 and name CB) (segid 3A4 and resid 279 and name CA)	6.13	0.12	0.13
	assign (segid 3A4 and resid 274 and name CB) (segid 3A4 and resid 279 and name CB)	9.69	0.10	0.09
55	assign (segid 3A4 and resid 274 and name CB) (segid 3A4 and resid 279 and name N)	9.76	0.16	0.15
	assign (segid 3A4 and resid 274 and name CB) (segid 3A4 and resid 280 and name CA)	11.10	0.17	0.18
	assign (segid 3A4 and resid 274 and name CB) (segid 3A4 and resid 280 and name CB)	10.78	0.30	0.29
	assign (segid 3A4 and resid 274 and name CB) (segid 3A4 and resid 281 and name CA)	11.34	0.14	0.13
	assign (segid 3A4 and resid 274 and name CB) (segid 3A4 and resid 281 and name CB)	10.39	0.12	0.12
	assign (segid 3A4 and resid 274 and name CB) (segid 3A4 and resid 282 and name CA)	13.02	0.14	0.15
60	assign (segid 3A4 and resid 274 and name CB) (segid 3A4 and resid 303 and name CA)	19.06	0.27	0.26
	assign (segid 3A4 and resid 274 and name CB) (segid 3A4 and resid 304 and name CA)	16.13	0.40	0.40
	assign (segid 3A4 and resid 274 and name CB) (segid 3A4 and resid 304 and name CB)	14.99	0.34	0.35
	assign (segid 3A4 and resid 274 and name CB) (segid 3A4 and resid 305 and name CA)	15.92	0.59	0.59
	assign (segid 3A4 and resid 274 and name CB) (segid 3A4 and resid 305 and name CB)	16.40	0.58	0.58
65	assign (segid 3A4 and resid 274 and name CB) (segid 3A4 and resid 307 and name CA)	17.69	0.63	0.64
	assign (segid 3A4 and resid 274 and name CB) (segid 3A4 and resid 307 and name CB)	17.38	0.70	0.70
	assign (segid 3A4 and resid 274 and name CB) (segid 3A4 and resid 308 and name CA)	14.60	0.56	0.56
	assign (segid 3A4 and resid 274 and name CB) (segid 3A4 and resid 308 and name CB)	13.60	0.60	0.61
	assign (segid 3A4 and resid 274 and name CB) (segid 3A4 and resid 309 and name CA)	17.18	0.64	0.65
70	assign (segid 3A4 and resid 274 and name CB) (segid 3A4 and resid 309 and name CB)	18.23	0.70	0.70
	assign (segid 3A4 and resid 274 and name CB) (segid 3A4 and resid 311 and name CA)	16.87	0.45	0.45
	assign (segid 3A4 and resid 274 and name CB) (segid 3A4 and resid 311 and name CB)	15.72	0.48	0.48
	assign (segid 3A4 and resid 274 and name CB) (segid 3A4 and resid 312 and name CA)	16.05	0.44	0.43
	assign (segid 3A4 and resid 274 and name CB) (segid 3A4 and resid 312 and name CB)	15.64	0.45	0.45
75	assign (segid 3A4 and resid 274 and name CB) (segid 3A4 and resid 315 and name CA)	17.95	0.48	0.48
	assign (segid 3A4 and resid 274 and name CB) (segid 3A4 and resid 315 and name CB)	16.46	0.48	0.48
	assign (segid 3A4 and resid 274 and name CB) (segid 3A4 and resid 359 and name CB)	18.85	0.65	0.65
	assign (segid 3A4 and resid 274 and name CB) (segid 3A4 and resid 361 and name CA)	17.91	0.60	0.60
	assign (segid 3A4 and resid 274 and name CB) (segid 3A4 and resid 362 and name CA)	14.84	0.60	0.60
80	assign (segid 3A4 and resid 274 and name CB) (segid 3A4 and resid 362 and name CB)	14.97	0.70	0.70
	assign (segid 3A4 and resid 274 and name CB) (segid 3A4 and resid 363 and name CA)	12.81	0.46	0.47
	assign (segid 3A4 and resid 274 and name CB) (segid 3A4 and resid 363 and name CB)	11.82	0.47	0.46
	assign (segid 3A4 and resid 274 and name CB) (segid 3A4 and resid 364 and name CA)	13.21	0.62	0.61

	assign (segid 3A4 and resid 274 and name CB)	(segid 3A4 and resid 364 and name CB)	14.10	0.67	0.66
	assign (segid 3A4 and resid 274 and name CB)	(segid 3A4 and resid 365 and name CA)	13.82	0.58	0.58
	assign (segid 3A4 and resid 274 and name CB)	(segid 3A4 and resid 365 and name CB)	12.94	0.59	0.58
	assign (segid 3A4 and resid 274 and name CB)	(segid 3A4 and resid 405 and name CA)	15.74	0.47	0.46
5	assign (segid 3A4 and resid 274 and name CB)	(segid 3A4 and resid 405 and name CB)	15.31	0.37	0.37
	assign (segid 3A4 and resid 274 and name CB)	(segid 3A4 and resid 406 and name CA)	16.72	0.65	0.66
	assign (segid 3A4 and resid 274 and name CB)	(segid 3A4 and resid 407 and name CA)	18.08	0.53	0.53
	assign (segid 3A4 and resid 274 and name CB)	(segid 3A4 and resid 407 and name CB)	19.39	0.47	0.47
	assign (segid 3A4 and resid 274 and name CB)	(segid 3A4 and resid 408 and name CA)	15.54	0.49	0.49
	assign (segid 3A4 and resid 274 and name CB)	(segid 3A4 and resid 408 and name CB)	15.05	0.46	0.45
10	assign (segid 3A4 and resid 274 and name CB)	(segid 3A4 and resid 409 and name CA)	12.68	0.49	0.49
	assign (segid 3A4 and resid 274 and name CB)	(segid 3A4 and resid 409 and name CB)	11.95	0.45	0.46
	assign (segid 3A4 and resid 274 and name CB)	(segid 3A4 and resid 410 and name CA)	15.23	0.57	0.57
	assign (segid 3A4 and resid 274 and name CB)	(segid 3A4 and resid 411 and name CA)	16.37	0.89	0.90
	assign (segid 3A4 and resid 274 and name CB)	(segid 3A4 and resid 411 and name CB)	17.33	0.84	0.84
15	assign (segid 3A4 and resid 274 and name CB)	(segid 3A4 and resid 412 and name CA)	13.47	1.13	1.13
	assign (segid 3A4 and resid 274 and name CB)	(segid 3A4 and resid 413 and name CA)	9.90	1.36	1.37
	assign (segid 3A4 and resid 274 and name CB)	(segid 3A4 and resid 414 and name CA)	9.63	1.34	1.34
	assign (segid 3A4 and resid 274 and name CB)	(segid 3A4 and resid 415 and name CA)	9.66	1.16	1.17
	assign (segid 3A4 and resid 274 and name CB)	(segid 3A4 and resid 415 and name CB)	9.89	1.16	1.15
20	assign (segid 3A4 and resid 274 and name CB)	(segid 3A4 and resid 416 and name CA)	11.43	1.44	1.44
	assign (segid 3A4 and resid 274 and name CB)	(segid 3A4 and resid 417 and name CA)	14.05	0.94	0.93
	assign (segid 3A4 and resid 274 and name CB)	(segid 3A4 and resid 423 and name CA)	16.56	1.22	1.22
	assign (segid 3A4 and resid 274 and name CB)	(segid 3A4 and resid 424 and name CA)	16.77	1.25	1.25
	assign (segid 3A4 and resid 274 and name CB)	(segid 3A4 and resid 438 and name CA)	16.91	0.80	0.79
25	assign (segid 3A4 and resid 274 and name CB)	(segid 3A4 and resid 439 and name CA)	16.69	0.77	0.77
	assign (segid 3A4 and resid 274 and name CB)	(segid 3A4 and resid 440 and name CA)	14.08	0.84	0.83
	assign (segid 3A4 and resid 274 and name CB)	(segid 3A4 and resid 274 and name C)	2.51	0.03	0.03
	assign (segid 3A4 and resid 274 and name N)	(segid 3A4 and resid 274 and name CA)	1.46	0.00	0.01
30	assign (segid 3A4 and resid 274 and name N)	(segid 3A4 and resid 274 and name CB)	2.34	0.01	0.01
	assign (segid 3A4 and resid 274 and name N)	(segid 3A4 and resid 275 and name C)	3.59	0.05	0.04
	assign (segid 3A4 and resid 274 and name N)	(segid 3A4 and resid 275 and name CA)	4.86	0.05	0.06
	assign (segid 3A4 and resid 274 and name N)	(segid 3A4 and resid 275 and name CB)	5.02	0.08	0.07
	assign (segid 3A4 and resid 274 and name N)	(segid 3A4 and resid 275 and name N)	2.86	0.04	0.04
35	assign (segid 3A4 and resid 274 and name N)	(segid 3A4 and resid 275 and name O)	5.99	0.07	0.08
	assign (segid 3A4 and resid 274 and name N)	(segid 3A4 and resid 276 and name C)	5.77	0.09	0.09
	assign (segid 3A4 and resid 274 and name N)	(segid 3A4 and resid 276 and name CA)	5.47	0.07	0.07
	assign (segid 3A4 and resid 274 and name N)	(segid 3A4 and resid 276 and name CB)	5.54	0.11	0.12
	assign (segid 3A4 and resid 274 and name N)	(segid 3A4 and resid 276 and name CG2)	5.93	0.22	0.21
40	assign (segid 3A4 and resid 274 and name N)	(segid 3A4 and resid 276 and name N)	4.43	0.06	0.05
	assign (segid 3A4 and resid 274 and name N)	(segid 3A4 and resid 276 and name O)	6.98	0.09	0.09
	assign (segid 3A4 and resid 274 and name N)	(segid 3A4 and resid 277 and name C)	6.60	0.16	0.16
	assign (segid 3A4 and resid 274 and name N)	(segid 3A4 and resid 277 and name CA)	5.71	0.17	0.17
	assign (segid 3A4 and resid 274 and name N)	(segid 3A4 and resid 277 and name CB)	5.11	0.23	0.23
45	assign (segid 3A4 and resid 274 and name N)	(segid 3A4 and resid 277 and name N)	4.95	0.13	0.13
	assign (segid 3A4 and resid 274 and name N)	(segid 3A4 and resid 278 and name CA)	7.36	0.12	0.12
	assign (segid 3A4 and resid 274 and name N)	(segid 3A4 and resid 278 and name CB)	7.13	0.09	0.10
	assign (segid 3A4 and resid 274 and name N)	(segid 3A4 and resid 278 and name N)	6.25	0.14	0.14
	assign (segid 3A4 and resid 274 and name N)	(segid 3A4 and resid 274 and name CB)	3.27	0.09	0.09
50	assign (segid 3A4 and resid 274 and name O)	(segid 3A4 and resid 275 and name C)	2.98	0.06	0.05
	assign (segid 3A4 and resid 274 and name O)	(segid 3A4 and resid 275 and name CA)	2.74	0.06	0.05
	assign (segid 3A4 and resid 274 and name O)	(segid 3A4 and resid 275 and name CB)	4.21	0.06	0.07
	assign (segid 3A4 and resid 274 and name O)	(segid 3A4 and resid 275 and name N)	2.24	0.01	0.01
	assign (segid 3A4 and resid 274 and name O)	(segid 3A4 and resid 275 and name O)	3.55	0.10	0.10
55	assign (segid 3A4 and resid 274 and name O)	(segid 3A4 and resid 276 and name C)	4.07	0.09	0.10
	assign (segid 3A4 and resid 274 and name O)	(segid 3A4 and resid 276 and name CA)	4.33	0.06	0.07
	assign (segid 3A4 and resid 274 and name O)	(segid 3A4 and resid 276 and name CB)	5.33	0.08	0.09
	assign (segid 3A4 and resid 274 and name O)	(segid 3A4 and resid 276 and name CG2)	6.14	0.12	0.13
	assign (segid 3A4 and resid 274 and name O)	(segid 3A4 and resid 276 and name N)	3.36	0.05	0.04
60	assign (segid 3A4 and resid 274 and name O)	(segid 3A4 and resid 276 and name O)	4.97	0.11	0.11
	assign (segid 3A4 and resid 274 and name O)	(segid 3A4 and resid 277 and name C)	3.87	0.12	0.11
	assign (segid 3A4 and resid 274 and name O)	(segid 3A4 and resid 277 and name CA)	3.76	0.10	0.10
	assign (segid 3A4 and resid 274 and name O)	(segid 3A4 and resid 277 and name CB)	3.61	0.08	0.07
	assign (segid 3A4 and resid 274 and name O)	(segid 3A4 and resid 277 and name N)	3.30	0.10	0.09
65	assign (segid 3A4 and resid 274 and name O)	(segid 3A4 and resid 277 and name O)	5.04	0.11	0.12
	assign (segid 3A4 and resid 274 and name O)	(segid 3A4 and resid 278 and name C)	5.07	0.09	0.10
	assign (segid 3A4 and resid 274 and name O)	(segid 3A4 and resid 278 and name CA)	3.89	0.12	0.11
	assign (segid 3A4 and resid 274 and name O)	(segid 3A4 and resid 278 and name CB)	3.58	0.09	0.08
	assign (segid 3A4 and resid 274 and name O)	(segid 3A4 and resid 278 and name N)	3.03	0.12	0.12
70	assign (segid 3A4 and resid 274 and name O)	(segid 3A4 and resid 278 and name O)	6.20	0.10	0.10
	assign (segid 3A4 and resid 274 and name O)	(segid 3A4 and resid 279 and name C)	7.30	0.09	0.09
	assign (segid 3A4 and resid 274 and name O)	(segid 3A4 and resid 279 and name CA)	6.44	0.10	0.11
	assign (segid 3A4 and resid 274 and name O)	(segid 3A4 and resid 279 and name CB)	6.61	0.14	0.14
	assign (segid 3A4 and resid 274 and name O)	(segid 3A4 and resid 279 and name N)	5.08	0.10	0.11
75	assign (segid 3A4 and resid 274 and name O)	(segid 3A4 and resid 280 and name N)	6.95	0.10	0.11
	assign (segid 3A4 and resid 274 and name O)	(segid 3A4 and resid 281 and name N)	7.76	0.10	0.09
	assign (segid 3A4 and resid 275 and name C)	(segid 3A4 and resid 275 and name CB)	2.49	0.03	0.03
	assign (segid 3A4 and resid 275 and name C)	(segid 3A4 and resid 275 and name O)	1.23	0.00	0.01
80	assign (segid 3A4 and resid 275 and name C)	(segid 3A4 and resid 276 and name C)	3.08	0.06	0.06
	assign (segid 3A4 and resid 275 and name C)	(segid 3A4 and resid 276 and name CA)	2.44	0.02	0.02
	assign (segid 3A4 and resid 275 and name C)	(segid 3A4 and resid 276 and name CB)	3.71	0.02	0.01
	assign (segid 3A4 and resid 275 and name C)	(segid 3A4 and resid 276 and name CG2)	4.09	0.11	0.12

	assign (segid 3A4 and resid 275 and name C)	(segid 3A4 and resid 276 and name N)	1.33	0.01	0.01
	assign (segid 3A4 and resid 275 and name C)	(segid 3A4 and resid 276 and name O)	3.90	0.09	0.09
	assign (segid 3A4 and resid 275 and name C)	(segid 3A4 and resid 277 and name C)	4.65	0.05	0.06
	assign (segid 3A4 and resid 275 and name C)	(segid 3A4 and resid 277 and name CA)	4.56	0.07	0.06
	assign (segid 3A4 and resid 275 and name C)	(segid 3A4 and resid 277 and name CB)	5.27	0.06	0.07
5	assign (segid 3A4 and resid 275 and name C)	(segid 3A4 and resid 277 and name N)	3.38	0.06	0.06
	assign (segid 3A4 and resid 275 and name C)	(segid 3A4 and resid 277 and name O)	5.73	0.05	0.04
	assign (segid 3A4 and resid 275 and name C)	(segid 3A4 and resid 278 and name C)	4.97	0.08	0.09
	assign (segid 3A4 and resid 275 and name C)	(segid 3A4 and resid 278 and name CA)	4.59	0.08	0.08
	assign (segid 3A4 and resid 275 and name C)	(segid 3A4 and resid 278 and name CB)	4.31	0.10	0.11
10	assign (segid 3A4 and resid 275 and name C)	(segid 3A4 and resid 278 and name N)	3.89	0.07	0.07
	assign (segid 3A4 and resid 275 and name C)	(segid 3A4 and resid 278 and name O)	6.18	0.09	0.09
	assign (segid 3A4 and resid 275 and name C)	(segid 3A4 and resid 279 and name C)	6.25	0.11	0.12
	assign (segid 3A4 and resid 275 and name C)	(segid 3A4 and resid 279 and name CA)	5.15	0.14	0.13
	assign (segid 3A4 and resid 275 and name C)	(segid 3A4 and resid 279 and name CB)	4.67	0.19	0.19
15	assign (segid 3A4 and resid 275 and name C)	(segid 3A4 and resid 279 and name N)	4.24	0.11	0.10
	assign (segid 3A4 and resid 275 and name C)	(segid 3A4 and resid 279 and name O)	7.42	0.12	0.11
	assign (segid 3A4 and resid 275 and name C)	(segid 3A4 and resid 280 and name CA)	7.43	0.13	0.12
	assign (segid 3A4 and resid 275 and name C)	(segid 3A4 and resid 280 and name CB)	7.48	0.17	0.16
	assign (segid 3A4 and resid 275 and name C)	(segid 3A4 and resid 280 and name N)	6.14	0.12	0.11
20	assign (segid 3A4 and resid 275 and name C)	(segid 3A4 and resid 275 and name C)	1.53	0.01	0.00
	assign (segid 3A4 and resid 275 and name CA)	(segid 3A4 and resid 275 and name CB)	1.52	0.02	0.02
	assign (segid 3A4 and resid 275 and name CA)	(segid 3A4 and resid 275 and name O)	2.40	0.01	0.02
	assign (segid 3A4 and resid 275 and name CA)	(segid 3A4 and resid 276 and name C)	4.43	0.04	0.05
	assign (segid 3A4 and resid 275 and name CA)	(segid 3A4 and resid 276 and name CA)	3.80	0.01	0.01
25	assign (segid 3A4 and resid 275 and name CA)	(segid 3A4 and resid 276 and name CB)	4.84	0.04	0.04
	assign (segid 3A4 and resid 275 and name CA)	(segid 3A4 and resid 276 and name CG2)	5.01	0.15	0.16
	assign (segid 3A4 and resid 275 and name CA)	(segid 3A4 and resid 276 and name N)	2.42	0.01	0.01
	assign (segid 3A4 and resid 275 and name CA)	(segid 3A4 and resid 276 and name O)	5.34	0.09	0.08
	assign (segid 3A4 and resid 275 and name CA)	(segid 3A4 and resid 277 and name C)	5.57	0.06	0.07
30	assign (segid 3A4 and resid 275 and name CA)	(segid 3A4 and resid 277 and name CB)	5.49	0.07	0.06
	assign (segid 3A4 and resid 275 and name CA)	(segid 3A4 and resid 277 and name N)	4.42	0.05	0.04
	assign (segid 3A4 and resid 275 and name CA)	(segid 3A4 and resid 277 and name O)	6.71	0.06	0.06
	assign (segid 3A4 and resid 275 and name CA)	(segid 3A4 and resid 278 and name C)	5.84	0.06	0.07
35	assign (segid 3A4 and resid 275 and name CA)	(segid 3A4 and resid 278 and name CA)	5.20	0.07	0.07
	assign (segid 3A4 and resid 275 and name CA)	(segid 3A4 and resid 278 and name CB)	4.53	0.10	0.10
	assign (segid 3A4 and resid 275 and name CA)	(segid 3A4 and resid 278 and name N)	4.63	0.07	0.07
	assign (segid 3A4 and resid 275 and name CA)	(segid 3A4 and resid 278 and name O)	7.03	0.07	0.07
	assign (segid 3A4 and resid 275 and name CA)	(segid 3A4 and resid 279 and name C)	7.54	0.10	0.10
40	assign (segid 3A4 and resid 275 and name CA)	(segid 3A4 and resid 279 and name CA)	6.34	0.11	0.11
	assign (segid 3A4 and resid 275 and name CA)	(segid 3A4 and resid 279 and name CB)	5.97	0.17	0.17
	assign (segid 3A4 and resid 275 and name CA)	(segid 3A4 and resid 279 and name N)	5.32	0.09	0.09
	assign (segid 3A4 and resid 275 and name CA)	(segid 3A4 and resid 280 and name CA)	8.79	0.10	0.11
	assign (segid 3A4 and resid 275 and name CA)	(segid 3A4 and resid 280 and name CB)	8.86	0.16	0.15
45	assign (segid 3A4 and resid 275 and name CA)	(segid 3A4 and resid 280 and name N)	7.49	0.10	0.09
	assign (segid 3A4 and resid 275 and name CA)	(segid 3A4 and resid 281 and name CA)	9.99	0.06	0.07
	assign (segid 3A4 and resid 275 and name CA)	(segid 3A4 and resid 281 and name CB)	9.52	0.05	0.06
	assign (segid 3A4 and resid 275 and name CA)	(segid 3A4 and resid 281 and name N)	10.72	0.07	0.06
	assign (segid 3A4 and resid 275 and name CA)	(segid 3A4 and resid 303 and name CA)	16.01	0.16	0.17
50	assign (segid 3A4 and resid 275 and name CA)	(segid 3A4 and resid 303 and name CB)	16.54	0.19	0.19
	assign (segid 3A4 and resid 275 and name CA)	(segid 3A4 and resid 304 and name CA)	12.92	0.41	0.42
	assign (segid 3A4 and resid 275 and name CA)	(segid 3A4 and resid 304 and name CB)	11.64	0.32	0.32
	assign (segid 3A4 and resid 275 and name CA)	(segid 3A4 and resid 305 and name CA)	13.62	0.61	0.61
	assign (segid 3A4 and resid 275 and name CA)	(segid 3A4 and resid 305 and name CB)	14.37	0.64	0.64
55	assign (segid 3A4 and resid 275 and name CA)	(segid 3A4 and resid 306 and name CA)	16.54	0.56	0.55
	assign (segid 3A4 and resid 275 and name CA)	(segid 3A4 and resid 307 and name CA)	14.75	0.52	0.52
	assign (segid 3A4 and resid 275 and name CA)	(segid 3A4 and resid 307 and name CB)	14.13	0.61	0.62
	assign (segid 3A4 and resid 275 and name CA)	(segid 3A4 and resid 308 and name CA)	12.29	0.40	0.40
	assign (segid 3A4 and resid 275 and name CA)	(segid 3A4 and resid 308 and name CB)	11.45	0.49	0.48
60	assign (segid 3A4 and resid 275 and name CA)	(segid 3A4 and resid 309 and name CA)	15.53	0.51	0.50
	assign (segid 3A4 and resid 275 and name CA)	(segid 3A4 and resid 309 and name CB)	16.61	0.54	0.55
	assign (segid 3A4 and resid 275 and name CA)	(segid 3A4 and resid 310 and name CA)	17.20	0.36	0.36
	assign (segid 3A4 and resid 275 and name CA)	(segid 3A4 and resid 310 and name CB)	17.56	0.43	0.43
	assign (segid 3A4 and resid 275 and name CA)	(segid 3A4 and resid 311 and name CA)	14.72	0.23	0.24
65	assign (segid 3A4 and resid 275 and name CA)	(segid 3A4 and resid 311 and name CB)	13.37	0.25	0.24
	assign (segid 3A4 and resid 275 and name CA)	(segid 3A4 and resid 312 and name CA)	14.91	0.36	0.36
	assign (segid 3A4 and resid 275 and name CA)	(segid 3A4 and resid 312 and name CB)	14.71	0.46	0.47
	assign (segid 3A4 and resid 275 and name CA)	(segid 3A4 and resid 313 and name CA)	18.67	0.34	0.34
	assign (segid 3A4 and resid 275 and name CA)	(segid 3A4 and resid 314 and name CA)	18.75	0.25	0.24
70	assign (segid 3A4 and resid 275 and name CA)	(segid 3A4 and resid 314 and name CB)	18.20	0.22	0.23
	assign (segid 3A4 and resid 275 and name CA)	(segid 3A4 and resid 315 and name CA)	16.88	0.50	0.50
	assign (segid 3A4 and resid 275 and name CA)	(segid 3A4 and resid 315 and name CB)	15.39	0.53	0.53
	assign (segid 3A4 and resid 275 and name CA)	(segid 3A4 and resid 359 and name CA)	17.48	0.51	0.52
	assign (segid 3A4 and resid 275 and name CA)	(segid 3A4 and resid 359 and name CB)	16.39	0.56	0.56
75	assign (segid 3A4 and resid 275 and name CA)	(segid 3A4 and resid 360 and name CA)	18.14	0.45	0.45
	assign (segid 3A4 and resid 275 and name CA)	(segid 3A4 and resid 361 and name CA)	16.67	0.65	0.64
	assign (segid 3A4 and resid 275 and name CA)	(segid 3A4 and resid 361 and name CB)	17.39	0.71	0.72
	assign (segid 3A4 and resid 275 and name CA)	(segid 3A4 and resid 362 and name CA)	13.13	0.59	0.58
	assign (segid 3A4 and resid 275 and name CA)	(segid 3A4 and resid 362 and name CB)	12.94	0.61	0.61
80	assign (segid 3A4 and resid 275 and name CA)	(segid 3A4 and resid 363 and name CA)	11.02	0.38	0.38
	assign (segid 3A4 and resid 275 and name CA)	(segid 3A4 and resid 363 and name CB)	10.44	0.33	0.34
	assign (segid 3A4 and resid 275 and name CA)	(segid 3A4 and resid 364 and name CA)	10.21	0.44	0.44

	assign (segid 3A4 and resid 275 and name CA)	(segid 3A4 and resid 364 and name CB)	10.94	0.53	0.52
	assign (segid 3A4 and resid 275 and name CA)	(segid 3A4 and resid 365 and name CA)	10.59	0.38	0.39
	assign (segid 3A4 and resid 275 and name CA)	(segid 3A4 and resid 365 and name CB)	9.75	0.38	0.37
	assign (segid 3A4 and resid 275 and name CA)	(segid 3A4 and resid 402 and name CA)	18.52	0.28	0.27
5	assign (segid 3A4 and resid 275 and name CA)	(segid 3A4 and resid 402 and name CB)	19.19	0.25	0.25
	assign (segid 3A4 and resid 275 and name CA)	(segid 3A4 and resid 405 and name CA)	15.57	0.47	0.48
	assign (segid 3A4 and resid 275 and name CA)	(segid 3A4 and resid 405 and name CB)	14.88	0.40	0.39
	assign (segid 3A4 and resid 275 and name CA)	(segid 3A4 and resid 406 and name CA)	16.06	0.51	0.51
	assign (segid 3A4 and resid 275 and name CA)	(segid 3A4 and resid 407 and name CA)	18.22	0.46	0.45
	assign (segid 3A4 and resid 275 and name CA)	(segid 3A4 and resid 408 and name CA)	16.46	0.41	0.40
10	assign (segid 3A4 and resid 275 and name CA)	(segid 3A4 and resid 408 and name CB)	16.08	0.39	0.40
	assign (segid 3A4 and resid 275 and name CA)	(segid 3A4 and resid 409 and name CA)	13.26	0.45	0.45
	assign (segid 3A4 and resid 275 and name CA)	(segid 3A4 and resid 409 and name CB)	12.16	0.35	0.35
	assign (segid 3A4 and resid 275 and name CA)	(segid 3A4 and resid 410 and name CA)	15.49	0.46	0.47
	assign (segid 3A4 and resid 275 and name CA)	(segid 3A4 and resid 411 and name CA)	17.57	0.74	0.74
15	assign (segid 3A4 and resid 275 and name CA)	(segid 3A4 and resid 411 and name CB)	18.61	0.65	0.64
	assign (segid 3A4 and resid 275 and name CA)	(segid 3A4 and resid 412 and name CA)	15.41	1.02	1.01
	assign (segid 3A4 and resid 275 and name CA)	(segid 3A4 and resid 413 and name CA)	12.77	1.14	1.15
	assign (segid 3A4 and resid 275 and name CA)	(segid 3A4 and resid 414 and name CA)	12.95	1.02	1.03
	assign (segid 3A4 and resid 275 and name CA)	(segid 3A4 and resid 415 and name CA)	13.56	0.85	0.84
20	assign (segid 3A4 and resid 275 and name CA)	(segid 3A4 and resid 415 and name CB)	13.86	0.82	0.82
	assign (segid 3A4 and resid 275 and name CA)	(segid 3A4 and resid 416 and name CA)	15.42	1.25	1.25
	assign (segid 3A4 and resid 275 and name CA)	(segid 3A4 and resid 417 and name CA)	18.27	0.73	0.74
	assign (segid 3A4 and resid 275 and name CA)	(segid 3A4 and resid 440 and name CA)	17.71	0.59	0.59
	assign (segid 3A4 and resid 275 and name CA)	(segid 3A4 and resid 276 and name C)	5.48	0.04	0.04
25	assign (segid 3A4 and resid 275 and name CB)	(segid 3A4 and resid 276 and name CA)	4.50	0.01	0.02
	assign (segid 3A4 and resid 275 and name CB)	(segid 3A4 and resid 276 and name CB)	5.34	0.06	0.05
	assign (segid 3A4 and resid 275 and name CB)	(segid 3A4 and resid 276 and name CG2)	5.07	0.16	0.17
	assign (segid 3A4 and resid 275 and name CB)	(segid 3A4 and resid 276 and name N)	3.19	0.02	0.01
	assign (segid 3A4 and resid 275 and name CB)	(segid 3A4 and resid 276 and name O)	6.34	0.09	0.08
30	assign (segid 3A4 and resid 275 and name CB)	(segid 3A4 and resid 277 and name C)	6.99	0.06	0.06
	assign (segid 3A4 and resid 275 and name CB)	(segid 3A4 and resid 277 and name CA)	6.86	0.05	0.06
	assign (segid 3A4 and resid 275 and name CB)	(segid 3A4 and resid 277 and name CB)	7.29	0.07	0.06
	assign (segid 3A4 and resid 275 and name CB)	(segid 3A4 and resid 277 and name N)	5.67	0.04	0.04
	assign (segid 3A4 and resid 275 and name CB)	(segid 3A4 and resid 278 and name C)	7.00	0.11	0.12
35	assign (segid 3A4 and resid 275 and name CB)	(segid 3A4 and resid 278 and name CA)	6.53	0.09	0.10
	assign (segid 3A4 and resid 275 and name CB)	(segid 3A4 and resid 278 and name CB)	5.77	0.13	0.12
	assign (segid 3A4 and resid 275 and name CB)	(segid 3A4 and resid 278 and name N)	6.06	0.08	0.08
	assign (segid 3A4 and resid 275 and name CB)	(segid 3A4 and resid 279 and name CA)	7.14	0.17	0.16
	assign (segid 3A4 and resid 275 and name CB)	(segid 3A4 and resid 279 and name CB)	6.52	0.21	0.22
40	assign (segid 3A4 and resid 275 and name CB)	(segid 3A4 and resid 279 and name N)	6.33	0.14	0.14
	assign (segid 3A4 and resid 275 and name CB)	(segid 3A4 and resid 280 and name CA)	9.83	0.15	0.16
	assign (segid 3A4 and resid 275 and name CB)	(segid 3A4 and resid 280 and name CB)	9.95	0.18	0.17
	assign (segid 3A4 and resid 275 and name CB)	(segid 3A4 and resid 281 and name CA)	11.28	0.11	0.11
	assign (segid 3A4 and resid 275 and name CB)	(segid 3A4 and resid 281 and name CB)	10.89	0.09	0.08
45	assign (segid 3A4 and resid 275 and name CB)	(segid 3A4 and resid 282 and name CA)	11.72	0.12	0.12
	assign (segid 3A4 and resid 275 and name CB)	(segid 3A4 and resid 303 and name CA)	16.61	0.25	0.25
	assign (segid 3A4 and resid 275 and name CB)	(segid 3A4 and resid 303 and name CB)	17.06	0.34	0.33
	assign (segid 3A4 and resid 275 and name CB)	(segid 3A4 and resid 304 and name CA)	13.43	0.51	0.52
	assign (segid 3A4 and resid 275 and name CB)	(segid 3A4 and resid 304 and name CB)	12.13	0.39	0.40
50	assign (segid 3A4 and resid 275 and name CB)	(segid 3A4 and resid 305 and name CA)	14.40	0.66	0.65
	assign (segid 3A4 and resid 275 and name CB)	(segid 3A4 and resid 305 and name CB)	15.26	0.68	0.67
	assign (segid 3A4 and resid 275 and name CB)	(segid 3A4 and resid 306 and name CA)	17.10	0.59	0.59
	assign (segid 3A4 and resid 275 and name CB)	(segid 3A4 and resid 307 and name CA)	15.02	0.56	0.56
	assign (segid 3A4 and resid 275 and name CB)	(segid 3A4 and resid 307 and name CB)	14.33	0.67	0.66
55	assign (segid 3A4 and resid 275 and name CB)	(segid 3A4 and resid 308 and name CA)	12.74	0.42	0.43
	assign (segid 3A4 and resid 275 and name CB)	(segid 3A4 and resid 308 and name CB)	12.05	0.52	0.53
	assign (segid 3A4 and resid 275 and name CB)	(segid 3A4 and resid 309 and name CA)	16.08	0.50	0.51
	assign (segid 3A4 and resid 275 and name CB)	(segid 3A4 and resid 309 and name CB)	17.24	0.54	0.54
	assign (segid 3A4 and resid 275 and name CB)	(segid 3A4 and resid 310 and name CA)	17.44	0.36	0.37
60	assign (segid 3A4 and resid 275 and name CB)	(segid 3A4 and resid 310 and name CB)	17.74	0.42	0.43
	assign (segid 3A4 and resid 275 and name CB)	(segid 3A4 and resid 311 and name CA)	14.78	0.25	0.25
	assign (segid 3A4 and resid 275 and name CB)	(segid 3A4 and resid 311 and name CB)	13.37	0.25	0.25
	assign (segid 3A4 and resid 275 and name CB)	(segid 3A4 and resid 312 and name CA)	15.22	0.40	0.39
	assign (segid 3A4 and resid 275 and name CB)	(segid 3A4 and resid 312 and name CB)	15.16	0.50	0.50
65	assign (segid 3A4 and resid 275 and name CB)	(segid 3A4 and resid 313 and name CA)	18.93	0.37	0.36
	assign (segid 3A4 and resid 275 and name CB)	(segid 3A4 and resid 314 and name CA)	18.70	0.28	0.27
	assign (segid 3A4 and resid 275 and name CB)	(segid 3A4 and resid 314 and name CB)	18.07	0.24	0.25
	assign (segid 3A4 and resid 275 and name CB)	(segid 3A4 and resid 315 and name CA)	16.77	0.55	0.56
	assign (segid 3A4 and resid 275 and name CB)	(segid 3A4 and resid 315 and name CB)	15.30	0.58	0.58
70	assign (segid 3A4 and resid 275 and name CB)	(segid 3A4 and resid 357 and name CB)	19.34	0.33	0.33
	assign (segid 3A4 and resid 275 and name CB)	(segid 3A4 and resid 358 and name CA)	18.85	0.52	0.52
	assign (segid 3A4 and resid 275 and name CB)	(segid 3A4 and resid 359 and name CA)	16.48	0.52	0.53
	assign (segid 3A4 and resid 275 and name CB)	(segid 3A4 and resid 359 and name CB)	15.33	0.58	0.57
	assign (segid 3A4 and resid 275 and name CB)	(segid 3A4 and resid 360 and name CA)	17.39	0.49	0.49
75	assign (segid 3A4 and resid 275 and name CB)	(segid 3A4 and resid 360 and name CB)	18.91	0.51	0.50
	assign (segid 3A4 and resid 275 and name CB)	(segid 3A4 and resid 361 and name CA)	15.98	0.70	0.71
	assign (segid 3A4 and resid 275 and name CB)	(segid 3A4 and resid 361 and name CB)	16.67	0.78	0.77
	assign (segid 3A4 and resid 275 and name CB)	(segid 3A4 and resid 362 and name CA)	12.37	0.63	0.63
	assign (segid 3A4 and resid 275 and name CB)	(segid 3A4 and resid 362 and name CB)	12.04	0.63	0.63
80	assign (segid 3A4 and resid 275 and name CB)	(segid 3A4 and resid 363 and name CA)	10.61	0.40	0.41
	assign (segid 3A4 and resid 275 and name CB)	(segid 3A4 and resid 363 and name CB)	10.20	0.37	0.36
	assign (segid 3A4 and resid 275 and name CB)	(segid 3A4 and resid 364 and name CA)	9.69	0.39	0.39

	assign (segid 3A4 and resid 275 and name CB)	(segid 3A4 and resid 364 and name CB)	10.24	0.49	0.48
	assign (segid 3A4 and resid 275 and name CB)	(segid 3A4 and resid 365 and name CA)	10.50	0.31	0.30
	assign (segid 3A4 and resid 275 and name CB)	(segid 3A4 and resid 365 and name CB)	9.84	0.31	0.30
	assign (segid 3A4 and resid 275 and name CB)	(segid 3A4 and resid 402 and name CA)	19.48	0.26	0.26
5	assign (segid 3A4 and resid 275 and name CB)	(segid 3A4 and resid 405 and name CA)	16.77	0.48	0.48
	assign (segid 3A4 and resid 275 and name CB)	(segid 3A4 and resid 405 and name CB)	15.99	0.40	0.40
	assign (segid 3A4 and resid 275 and name CB)	(segid 3A4 and resid 406 and name CA)	17.30	0.50	0.49
	assign (segid 3A4 and resid 275 and name CB)	(segid 3A4 and resid 408 and name CA)	17.87	0.39	0.40
	assign (segid 3A4 and resid 275 and name CB)	(segid 3A4 and resid 408 and name CB)	17.46	0.39	0.39
	assign (segid 3A4 and resid 275 and name CB)	(segid 3A4 and resid 409 and name CA)	14.72	0.46	0.45
10	assign (segid 3A4 and resid 275 and name CB)	(segid 3A4 and resid 409 and name CB)	13.58	0.35	0.35
	assign (segid 3A4 and resid 275 and name CB)	(segid 3A4 and resid 410 and name CA)	16.95	0.48	0.47
	assign (segid 3A4 and resid 275 and name CB)	(segid 3A4 and resid 412 and name CA)	16.91	1.02	1.02
	assign (segid 3A4 and resid 275 and name CB)	(segid 3A4 and resid 413 and name CA)	14.18	1.17	1.17
	assign (segid 3A4 and resid 275 and name CB)	(segid 3A4 and resid 414 and name CA)	14.25	1.09	1.07
15	assign (segid 3A4 and resid 275 and name CB)	(segid 3A4 and resid 415 and name CA)	14.64	0.80	0.80
	assign (segid 3A4 and resid 275 and name CB)	(segid 3A4 and resid 415 and name CB)	14.90	0.78	0.79
	assign (segid 3A4 and resid 275 and name CB)	(segid 3A4 and resid 416 and name CA)	16.33	1.19	1.19
	assign (segid 3A4 and resid 275 and name CB)	(segid 3A4 and resid 275 and name C)	2.45	0.02	0.02
	assign (segid 3A4 and resid 275 and name N)	(segid 3A4 and resid 275 and name CA)	1.45	0.00	0.01
20	assign (segid 3A4 and resid 275 and name N)	(segid 3A4 and resid 275 and name CB)	2.45	0.03	0.03
	assign (segid 3A4 and resid 275 and name N)	(segid 3A4 and resid 275 and name O)	3.53	0.03	0.02
	assign (segid 3A4 and resid 275 and name N)	(segid 3A4 and resid 276 and name C)	4.66	0.05	0.04
	assign (segid 3A4 and resid 275 and name N)	(segid 3A4 and resid 276 and name CA)	4.14	0.05	0.05
	assign (segid 3A4 and resid 275 and name N)	(segid 3A4 and resid 276 and name CB)	4.88	0.10	0.11
25	assign (segid 3A4 and resid 275 and name N)	(segid 3A4 and resid 276 and name CG2)	5.16	0.21	0.20
	assign (segid 3A4 and resid 275 and name N)	(segid 3A4 and resid 276 and name N)	2.73	0.05	0.04
	assign (segid 3A4 and resid 275 and name N)	(segid 3A4 and resid 276 and name O)	5.74	0.07	0.07
	assign (segid 3A4 and resid 275 and name N)	(segid 3A4 and resid 277 and name C)	5.65	0.07	0.07
	assign (segid 3A4 and resid 275 and name N)	(segid 3A4 and resid 277 and name CA)	5.29	0.07	0.07
30	assign (segid 3A4 and resid 275 and name N)	(segid 3A4 and resid 277 and name CB)	5.31	0.09	0.08
	assign (segid 3A4 and resid 275 and name N)	(segid 3A4 and resid 277 and name N)	4.28	0.05	0.04
	assign (segid 3A4 and resid 275 and name N)	(segid 3A4 and resid 277 and name O)	6.87	0.07	0.06
	assign (segid 3A4 and resid 275 and name N)	(segid 3A4 and resid 278 and name C)	6.55	0.03	0.04
35	assign (segid 3A4 and resid 275 and name N)	(segid 3A4 and resid 278 and name CA)	5.67	0.08	0.07
	assign (segid 3A4 and resid 275 and name N)	(segid 3A4 and resid 278 and name CB)	5.11	0.08	0.08
	assign (segid 3A4 and resid 275 and name N)	(segid 3A4 and resid 278 and name N)	4.86	0.07	0.06
	assign (segid 3A4 and resid 275 and name N)	(segid 3A4 and resid 278 and name O)	7.75	0.04	0.05
	assign (segid 3A4 and resid 275 and name N)	(segid 3A4 and resid 279 and name CA)	7.33	0.10	0.10
40	assign (segid 3A4 and resid 275 and name N)	(segid 3A4 and resid 279 and name CB)	7.06	0.17	0.17
	assign (segid 3A4 and resid 275 and name N)	(segid 3A4 and resid 279 and name N)	6.19	0.07	0.07
	assign (segid 3A4 and resid 275 and name O)	(segid 3A4 and resid 275 and name CB)	3.23	0.06	0.06
	assign (segid 3A4 and resid 275 and name O)	(segid 3A4 and resid 276 and name C)	3.13	0.10	0.09
	assign (segid 3A4 and resid 275 and name O)	(segid 3A4 and resid 276 and name CA)	2.79	0.04	0.03
45	assign (segid 3A4 and resid 275 and name O)	(segid 3A4 and resid 276 and name CB)	4.25	0.02	0.03
	assign (segid 3A4 and resid 275 and name O)	(segid 3A4 and resid 276 and name CG2)	4.73	0.12	0.12
	assign (segid 3A4 and resid 275 and name O)	(segid 3A4 and resid 276 and name N)	2.26	0.02	0.01
	assign (segid 3A4 and resid 275 and name O)	(segid 3A4 and resid 276 and name O)	3.57	0.15	0.15
	assign (segid 3A4 and resid 275 and name O)	(segid 3A4 and resid 277 and name C)	4.39	0.10	0.09
50	assign (segid 3A4 and resid 275 and name O)	(segid 3A4 and resid 277 and name CA)	4.64	0.10	0.11
	assign (segid 3A4 and resid 275 and name O)	(segid 3A4 and resid 277 and name CB)	5.58	0.08	0.08
	assign (segid 3A4 and resid 275 and name O)	(segid 3A4 and resid 277 and name N)	3.67	0.08	0.08
	assign (segid 3A4 and resid 275 and name O)	(segid 3A4 and resid 277 and name O)	5.30	0.08	0.07
	assign (segid 3A4 and resid 275 and name O)	(segid 3A4 and resid 278 and name C)	4.04	0.11	0.12
	assign (segid 3A4 and resid 275 and name O)	(segid 3A4 and resid 278 and name CA)	3.96	0.11	0.10
55	assign (segid 3A4 and resid 275 and name O)	(segid 3A4 and resid 278 and name CB)	3.72	0.13	0.13
	assign (segid 3A4 and resid 275 and name O)	(segid 3A4 and resid 278 and name N)	3.54	0.11	0.12
	assign (segid 3A4 and resid 275 and name O)	(segid 3A4 and resid 278 and name O)	5.21	0.11	0.10
	assign (segid 3A4 and resid 275 and name O)	(segid 3A4 and resid 279 and name C)	5.23	0.12	0.12
	assign (segid 3A4 and resid 275 and name O)	(segid 3A4 and resid 279 and name CA)	4.01	0.13	0.13
60	assign (segid 3A4 and resid 275 and name O)	(segid 3A4 and resid 279 and name CB)	3.59	0.17	0.17
	assign (segid 3A4 and resid 275 and name O)	(segid 3A4 and resid 279 and name N)	3.19	0.12	0.12
	assign (segid 3A4 and resid 275 and name O)	(segid 3A4 and resid 279 and name O)	6.34	0.12	0.12
	assign (segid 3A4 and resid 275 and name O)	(segid 3A4 and resid 280 and name C)	7.52	0.14	0.15
	assign (segid 3A4 and resid 275 and name O)	(segid 3A4 and resid 280 and name CA)	6.67	0.13	0.14
65	assign (segid 3A4 and resid 275 and name O)	(segid 3A4 and resid 280 and name CB)	6.95	0.17	0.16
	assign (segid 3A4 and resid 275 and name O)	(segid 3A4 and resid 280 and name N)	5.30	0.13	0.13
	assign (segid 3A4 and resid 275 and name O)	(segid 3A4 and resid 281 and name N)	7.17	0.13	0.13
	assign (segid 3A4 and resid 276 and name C)	(segid 3A4 and resid 276 and name CB)	2.51	0.01	0.01
	assign (segid 3A4 and resid 276 and name C)	(segid 3A4 and resid 276 and name CG2)	3.84	0.04	0.05
70	assign (segid 3A4 and resid 276 and name C)	(segid 3A4 and resid 276 and name O)	1.23	0.00	0.01
	assign (segid 3A4 and resid 276 and name C)	(segid 3A4 and resid 277 and name C)	3.00	0.02	0.01
	assign (segid 3A4 and resid 276 and name C)	(segid 3A4 and resid 277 and name CA)	2.44	0.02	0.01
	assign (segid 3A4 and resid 276 and name C)	(segid 3A4 and resid 277 and name CB)	3.71	0.03	0.02
	assign (segid 3A4 and resid 276 and name C)	(segid 3A4 and resid 277 and name N)	1.33	0.01	0.01
75	assign (segid 3A4 and resid 276 and name C)	(segid 3A4 and resid 277 and name O)	3.85	0.04	0.03
	assign (segid 3A4 and resid 276 and name C)	(segid 3A4 and resid 278 and name C)	4.54	0.05	0.05
	assign (segid 3A4 and resid 276 and name C)	(segid 3A4 and resid 278 and name CA)	4.42	0.05	0.04
	assign (segid 3A4 and resid 276 and name C)	(segid 3A4 and resid 278 and name CB)	5.13	0.06	0.05
	assign (segid 3A4 and resid 276 and name C)	(segid 3A4 and resid 278 and name N)	3.23	0.05	0.04
80	assign (segid 3A4 and resid 276 and name C)	(segid 3A4 and resid 278 and name O)	5.61	0.07	0.07
	assign (segid 3A4 and resid 276 and name C)	(segid 3A4 and resid 279 and name C)	4.91	0.10	0.09
	assign (segid 3A4 and resid 276 and name C)	(segid 3A4 and resid 279 and name CA)	4.55	0.10	0.09

	assign (segid 3A4 and resid 276 and name C)	(segid 3A4 and resid 279 and name CB)	4.25	0.20	0.21
	assign (segid 3A4 and resid 276 and name C)	(segid 3A4 and resid 279 and name N)	3.82	0.05	0.06
	assign (segid 3A4 and resid 276 and name C)	(segid 3A4 and resid 279 and name O)	6.12	0.09	0.10
	assign (segid 3A4 and resid 276 and name C)	(segid 3A4 and resid 280 and name C)	6.17	0.17	0.17
5	assign (segid 3A4 and resid 276 and name C)	(segid 3A4 and resid 280 and name CA)	5.12	0.16	0.15
	assign (segid 3A4 and resid 276 and name C)	(segid 3A4 and resid 280 and name CB)	4.75	0.20	0.19
	assign (segid 3A4 and resid 276 and name C)	(segid 3A4 and resid 280 and name N)	4.19	0.12	0.12
	assign (segid 3A4 and resid 276 and name C)	(segid 3A4 and resid 280 and name O)	7.34	0.16	0.16
	assign (segid 3A4 and resid 276 and name C)	(segid 3A4 and resid 281 and name CA)	7.27	0.15	0.15
	assign (segid 3A4 and resid 276 and name C)	(segid 3A4 and resid 281 and name CB)	7.26	0.12	0.12
10	assign (segid 3A4 and resid 276 and name C)	(segid 3A4 and resid 281 and name N)	6.00	0.15	0.15
	assign (segid 3A4 and resid 276 and name C)	(segid 3A4 and resid 308 and name CB)	7.35	0.39	0.39
	assign (segid 3A4 and resid 276 and name C)	(segid 3A4 and resid 365 and name CB)	6.86	0.65	0.65
	assign (segid 3A4 and resid 276 and name C)	(segid 3A4 and resid 276 and name C)	1.52	0.01	0.01
	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 276 and name CB)	1.54	0.02	0.01
15	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 276 and name CG2)	2.50	0.06	0.06
	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 276 and name O)	2.39	0.01	0.01
	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 277 and name C)	4.39	0.03	0.02
	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 277 and name CA)	3.80	0.03	0.03
	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 277 and name CB)	4.85	0.05	0.05
20	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 277 and name N)	2.42	0.02	0.03
	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 277 and name O)	5.30	0.05	0.05
	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 278 and name C)	5.48	0.09	0.09
	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 278 and name CA)	5.39	0.07	0.07
	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 278 and name CB)	5.76	0.07	0.08
25	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 278 and name N)	4.32	0.05	0.05
	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 278 and name O)	6.61	0.10	0.10
	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 279 and name C)	5.76	0.13	0.14
	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 279 and name CA)	5.14	0.15	0.15
	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 279 and name CB)	4.44	0.25	0.26
30	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 279 and name N)	4.56	0.11	0.11
	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 279 and name O)	6.95	0.11	0.12
	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 280 and name C)	7.45	0.18	0.18
	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 280 and name CA)	6.28	0.17	0.18
	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 280 and name CB)	5.99	0.21	0.20
35	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 280 and name N)	5.26	0.16	0.15
	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 281 and name CA)	8.66	0.15	0.14
	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 281 and name CB)	8.66	0.12	0.12
	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 281 and name N)	7.36	0.15	0.15
	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 282 and name CA)	9.96	0.13	0.13
40	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 303 and name CA)	13.16	0.23	0.23
	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 303 and name CB)	13.87	0.32	0.32
	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 304 and name CA)	9.84	0.45	0.45
	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 304 and name CB)	8.74	0.35	0.35
	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 305 and name CA)	10.16	0.61	0.60
45	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 305 and name CB)	11.01	0.61	0.61
	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 306 and name CA)	12.89	0.57	0.56
	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 307 and name CA)	11.17	0.54	0.54
	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 307 and name CB)	10.72	0.64	0.64
	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 308 and name CA)	8.53	0.40	0.40
50	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 308 and name CB)	7.69	0.50	0.50
	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 309 and name CA)	11.76	0.50	0.49
	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 309 and name CB)	12.84	0.54	0.54
	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 310 and name CA)	13.50	0.36	0.36
	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 310 and name CB)	13.90	0.42	0.42
55	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 311 and name CA)	11.28	0.24	0.24
	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 311 and name CB)	9.97	0.24	0.25
	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 312 and name CA)	11.50	0.39	0.39
	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 312 and name CB)	11.24	0.48	0.49
	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 313 and name CA)	15.21	0.35	0.34
60	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 313 and name CB)	15.94	0.34	0.33
	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 314 and name CA)	15.54	0.27	0.27
	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 314 and name CB)	15.03	0.24	0.24
	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 315 and name CA)	14.08	0.55	0.54
	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 315 and name CB)	12.65	0.59	0.60
65	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 316 and name CA)	15.82	0.63	0.63
	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 317 and name CA)	18.84	0.42	0.43
	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 357 and name CA)	18.48	0.42	0.42
	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 357 and name CB)	17.68	0.38	0.37
	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 358 and name CA)	18.33	0.62	0.62
70	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 359 and name CA)	16.29	0.43	0.44
	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 359 and name CB)	15.39	0.52	0.52
	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 360 and name CA)	16.30	0.43	0.44
	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 360 and name CB)	17.75	0.45	0.45
	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 361 and name CA)	15.19	0.64	0.63
75	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 361 and name CB)	16.15	0.69	0.70
	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 362 and name CA)	11.80	0.59	0.59
	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 362 and name CB)	11.85	0.60	0.60
	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 363 and name CA)	8.88	0.45	0.46
	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 363 and name CB)	8.27	0.44	0.43
80	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 364 and name CA)	7.89	0.55	0.56
	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 364 and name CB)	8.98	0.62	0.62
	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 365 and name CA)	7.42	0.54	0.55

	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 365 and name CB)	6.39	0.52	0.52
	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 365 and name N)	6.99	0.55	0.55
	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 398 and name CA)	18.74	0.15	0.14
	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 398 and name CB)	18.93	0.20	0.21
5	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 401 and name CA)	16.14	0.39	0.39
	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 402 and name CA)	15.01	0.26	0.26
	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 402 and name CB)	15.64	0.22	0.23
	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 403 and name CA)	17.26	0.34	0.34
	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 403 and name CB)	18.77	0.34	0.33
10	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 404 and name CA)	16.27	0.57	0.58
	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 404 and name CB)	16.50	0.70	0.71
	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 405 and name CA)	12.56	0.51	0.51
	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 405 and name CB)	11.66	0.44	0.44
	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 406 and name CA)	13.27	0.50	0.50
	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 407 and name CA)	15.85	0.45	0.46
15	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 407 and name CB)	17.18	0.40	0.40
	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 408 and name CA)	14.38	0.41	0.42
	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 408 and name CB)	13.89	0.41	0.42
	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 409 and name CA)	11.53	0.51	0.50
	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 409 and name CB)	10.24	0.43	0.42
20	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 410 and name CA)	14.05	0.40	0.45
	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 411 and name CA)	16.43	0.65	0.66
	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 411 and name CB)	17.29	0.56	0.57
	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 412 and name CA)	14.72	0.96	0.95
	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 413 and name CA)	13.05	1.14	1.15
25	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 414 and name CA)	12.87	0.93	0.93
	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 415 and name CA)	13.87	0.69	0.68
	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 415 and name CB)	14.44	0.65	0.66
	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 416 and name CA)	15.62	1.19	1.19
	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 438 and name CA)	18.74	0.35	0.34
30	assign (segid 3A4 and resid 276 and name CA)	(segid 3A4 and resid 440 and name CA)	17.24	0.50	0.51
	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 276 and name CG2)	1.52	0.02	0.01
	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 277 and name C)	5.42	0.03	0.02
	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 277 and name CA)	4.49	0.06	0.05
	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 277 and name CB)	5.36	0.10	0.10
35	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 277 and name N)	3.15	0.05	0.06
	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 277 and name O)	6.29	0.03	0.03
	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 278 and name C)	6.89	0.07	0.08
	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 278 and name CA)	6.77	0.05	0.06
	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 278 and name CB)	7.21	0.08	0.09
40	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 278 and name N)	5.58	0.05	0.05
	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 279 and name C)	6.90	0.13	0.13
	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 279 and name CA)	6.46	0.16	0.16
	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 279 and name CB)	5.66	0.28	0.29
	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 279 and name N)	5.99	0.10	0.10
45	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 280 and name CA)	7.04	0.19	0.19
	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 280 and name CB)	6.48	0.22	0.22
	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 280 and name N)	6.24	0.15	0.15
	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 281 and name CA)	9.67	0.17	0.16
	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 281 and name CB)	9.73	0.13	0.12
50	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 282 and name CA)	11.23	0.14	0.14
	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 303 and name CA)	13.51	0.34	0.33
	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 303 and name CB)	14.29	0.43	0.43
	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 304 and name CA)	10.07	0.51	0.50
	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 304 and name CB)	9.12	0.36	0.36
55	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 305 and name CA)	10.09	0.61	0.61
	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 305 and name CB)	11.02	0.60	0.59
	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 306 and name CA)	12.52	0.61	0.61
	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 307 and name CA)	10.67	0.60	0.59
60	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 307 and name CB)	10.36	0.70	0.69
	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 308 and name CA)	7.79	0.49	0.48
	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 308 and name CB)	7.09	0.58	0.58
	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 309 and name CA)	10.86	0.54	0.54
	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 309 and name CB)	12.04	0.58	0.59
65	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 310 and name CA)	12.50	0.40	0.40
	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 310 and name CB)	13.00	0.47	0.46
	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 311 and name CA)	10.09	0.27	0.26
	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 311 and name CB)	8.83	0.30	0.29
	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 312 and name CA)	10.15	0.40	0.40
70	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 312 and name CB)	9.96	0.52	0.52
	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 313 and name CA)	13.88	0.36	0.37
	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 313 and name CB)	14.69	0.36	0.35
	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 314 and name CA)	14.17	0.28	0.27
	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 314 and name CB)	13.71	0.25	0.25
	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 315 and name CA)	12.59	0.54	0.55
75	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 315 and name CB)	11.16	0.59	0.60
	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 316 and name CA)	14.32	0.64	0.64
	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 317 and name CA)	17.38	0.44	0.44
	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 318 and name CA)	19.23	0.34	0.35
	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 318 and name CB)	18.90	0.33	0.34
80	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 351 and name CA)	18.43	0.33	0.33
	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 352 and name CA)	18.25	0.48	0.47
	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 352 and name CB)	18.34	0.55	0.55

	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 357 and name CA)	17.41	0.42	0.12
	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 357 and name CB)	16.54	0.37	0.37
	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 358 and name CA)	17.39	0.61	0.61
	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 358 and name CB)	17.57	0.83	0.83
5	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 359 and name CA)	15.28	0.46	0.46
	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 359 and name CB)	14.46	0.54	0.54
	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 360 and name CA)	15.06	0.44	0.44
	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 360 and name CB)	16.48	0.45	0.46
	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 361 and name CA)	13.87	0.64	0.63
	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 361 and name CB)	14.85	0.70	0.71
10	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 362 and name CA)	10.62	0.60	0.59
	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 362 and name CB)	10.80	0.63	0.62
	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 363 and name C)	6.79	0.53	0.52
	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 363 and name CA)	7.54	0.47	0.47
	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 363 and name CB)	6.84	0.45	0.44
15	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 363 and name CG)	6.12	0.40	0.39
	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 363 and name O)	6.08	0.63	0.63
	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 364 and name CA)	6.94	0.62	0.63
	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 364 and name CB)	8.15	0.68	0.67
	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 364 and name N)	7.21	0.50	0.49
20	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 365 and name CA)	6.73	0.59	0.59
	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 365 and name CB)	5.83	0.56	0.56
	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 365 and name N)	6.18	0.63	0.63
	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 381 and name CA)	18.85	0.46	0.47
25	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 398 and name CA)	17.98	0.14	0.14
	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 398 and name CB)	18.19	0.17	0.18
	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 399 and name CA)	19.40	0.25	0.24
	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 400 and name CA)	19.09	0.44	0.43
	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 401 and name CA)	15.46	0.45	0.44
30	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 402 and name CA)	14.62	0.31	0.31
	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 402 and name CB)	15.29	0.27	0.26
	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 403 and name CA)	17.05	0.40	0.39
	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 403 and name CB)	18.53	0.39	0.39
	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 403 and name CB)	15.95	0.63	0.62
35	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 404 and name CA)	16.05	0.76	0.75
	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 405 and name CA)	12.29	0.54	0.55
	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 405 and name CB)	11.30	0.47	0.46
	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 406 and name CA)	13.40	0.57	0.57
	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 407 and name CA)	16.02	0.50	0.50
40	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 407 and name CB)	17.28	0.44	0.44
	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 408 and name CA)	14.45	0.43	0.43
	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 408 and name CB)	13.82	0.44	0.44
	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 409 and name CA)	11.89	0.51	0.51
	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 409 and name CB)	10.60	0.43	0.44
45	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 410 and name CA)	14.68	0.43	0.42
	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 411 and name CA)	16.94	0.62	0.62
	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 411 and name CB)	17.69	0.54	0.54
	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 412 and name CA)	15.17	0.93	0.94
	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 413 and name CA)	13.53	1.21	1.21
50	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 414 and name CA)	12.96	0.99	0.99
	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 415 and name CA)	13.76	0.66	0.65
	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 415 and name CB)	14.39	0.70	0.71
	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 416 and name CA)	15.24	1.15	1.15
	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 435 and name CA)	18.44	0.54	0.53
55	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 438 and name CA)	17.87	0.39	0.39
	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 439 and name CA)	18.93	0.45	0.45
	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 440 and name CA)	16.86	0.55	0.56
	assign (segid 3A4 and resid 276 and name CB)	(segid 3A4 and resid 277 and name C)	6.77	0.05	0.06
	assign (segid 3A4 and resid 276 and name CG2)	(segid 3A4 and resid 277 and name CA)	5.92	0.04	0.04
60	assign (segid 3A4 and resid 276 and name CG2)	(segid 3A4 and resid 277 and name CB)	6.73	0.08	0.08
	assign (segid 3A4 and resid 276 and name CG2)	(segid 3A4 and resid 277 and name N)	4.53	0.04	0.03
	assign (segid 3A4 and resid 276 and name CG2)	(segid 3A4 and resid 277 and name O)	7.67	0.06	0.07
	assign (segid 3A4 and resid 276 and name CG2)	(segid 3A4 and resid 278 and name N)	6.77	0.11	0.10
	assign (segid 3A4 and resid 276 and name CG2)	(segid 3A4 and resid 279 and name CA)	7.27	0.25	0.25
65	assign (segid 3A4 and resid 276 and name CG2)	(segid 3A4 and resid 279 and name CB)	6.25	0.36	0.35
	assign (segid 3A4 and resid 276 and name CG2)	(segid 3A4 and resid 279 and name N)	6.92	0.20	0.19
	assign (segid 3A4 and resid 276 and name CG2)	(segid 3A4 and resid 280 and name N)	7.37	0.22	0.21
	assign (segid 3A4 and resid 276 and name CG2)	(segid 3A4 and resid 363 and name C)	5.64	0.51	0.50
	assign (segid 3A4 and resid 276 and name CG2)	(segid 3A4 and resid 363 and name CA)	6.50	0.48	0.48
70	assign (segid 3A4 and resid 276 and name CG2)	(segid 3A4 and resid 363 and name CB)	5.98	0.48	0.48
	assign (segid 3A4 and resid 276 and name CG2)	(segid 3A4 and resid 363 and name CG)	5.51	0.46	0.46
	assign (segid 3A4 and resid 276 and name CG2)	(segid 3A4 and resid 363 and name O)	4.81	0.61	0.62
	assign (segid 3A4 and resid 276 and name CG2)	(segid 3A4 and resid 364 and name C)	6.20	0.49	0.48
	assign (segid 3A4 and resid 276 and name CG2)	(segid 3A4 and resid 364 and name CA)	5.82	0.54	0.54
	assign (segid 3A4 and resid 276 and name CG2)	(segid 3A4 and resid 364 and name N)	6.11	0.44	0.43
75	assign (segid 3A4 and resid 276 and name CG2)	(segid 3A4 and resid 365 and name CA)	6.30	0.41	0.42
	assign (segid 3A4 and resid 276 and name CG2)	(segid 3A4 and resid 365 and name CB)	5.71	0.39	0.38
	assign (segid 3A4 and resid 276 and name CG2)	(segid 3A4 and resid 365 and name N)	5.48	0.47	0.48
	assign (segid 3A4 and resid 276 and name CG2)	(segid 3A4 and resid 276 and name C)	2.45	0.03	0.02
80	assign (segid 3A4 and resid 276 and name N)	(segid 3A4 and resid 276 and name CA)	1.46	0.01	0.01
	assign (segid 3A4 and resid 276 and name N)	(segid 3A4 and resid 276 and name CB)	2.46	0.03	0.02
	assign (segid 3A4 and resid 276 and name N)	(segid 3A4 and resid 276 and name CG2)	2.96	0.10	0.10
	assign (segid 3A4 and resid 276 and name N)	(segid 3A4 and resid 276 and name O)	3.48	0.03	0.04

	assign (segid 3A4 and resid 276 and name N)	(segid 3A4 and resid 277 and name C)	4.67	0.03	0.03
	assign (segid 3A4 and resid 276 and name N)	(segid 3A4 and resid 277 and name CA)	4.17	0.04	0.05
	assign (segid 3A4 and resid 276 and name N)	(segid 3A4 and resid 277 and name CB)	4.89	0.07	0.07
	assign (segid 3A4 and resid 276 and name N)	(segid 3A4 and resid 277 and name N)	2.77	0.04	0.05
5	assign (segid 3A4 and resid 276 and name N)	(segid 3A4 and resid 277 and name O)	5.77	0.04	0.04
	assign (segid 3A4 and resid 276 and name N)	(segid 3A4 and resid 278 and name C)	5.63	0.09	0.09
	assign (segid 3A4 and resid 276 and name N)	(segid 3A4 and resid 278 and name CA)	5.26	0.07	0.07
	assign (segid 3A4 and resid 276 and name N)	(segid 3A4 and resid 278 and name CB)	5.28	0.10	0.09
	assign (segid 3A4 and resid 276 and name N)	(segid 3A4 and resid 278 and name N)	4.25	0.04	0.05
10	assign (segid 3A4 and resid 276 and name N)	(segid 3A4 and resid 278 and name O)	6.84	0.09	0.09
	assign (segid 3A4 and resid 276 and name N)	(segid 3A4 and resid 279 and name C)	6.54	0.13	0.13
	assign (segid 3A4 and resid 276 and name N)	(segid 3A4 and resid 279 and name CA)	5.67	0.15	0.15
	assign (segid 3A4 and resid 276 and name N)	(segid 3A4 and resid 279 and name CB)	5.08	0.24	0.23
	assign (segid 3A4 and resid 276 and name N)	(segid 3A4 and resid 279 and name N)	4.85	0.12	0.12
15	assign (segid 3A4 and resid 276 and name N)	(segid 3A4 and resid 279 and name O)	7.75	0.13	0.12
	assign (segid 3A4 and resid 276 and name N)	(segid 3A4 and resid 280 and name CA)	7.33	0.15	0.16
	assign (segid 3A4 and resid 276 and name N)	(segid 3A4 and resid 280 and name CB)	7.14	0.20	0.20
	assign (segid 3A4 and resid 276 and name N)	(segid 3A4 and resid 280 and name N)	6.19	0.14	0.13
	assign (segid 3A4 and resid 276 and name N)	(segid 3A4 and resid 276 and name CB)	3.31	0.05	0.04
20	assign (segid 3A4 and resid 276 and name O)	(segid 3A4 and resid 276 and name CG2)	4.58	0.08	0.07
	assign (segid 3A4 and resid 276 and name O)	(segid 3A4 and resid 277 and name C)	2.94	0.03	0.02
	assign (segid 3A4 and resid 276 and name O)	(segid 3A4 and resid 277 and name CA)	2.78	0.02	0.01
	assign (segid 3A4 and resid 276 and name O)	(segid 3A4 and resid 277 and name CB)	4.26	0.02	0.02
	assign (segid 3A4 and resid 276 and name O)	(segid 3A4 and resid 277 and name N)	2.25	0.02	0.02
25	assign (segid 3A4 and resid 276 and name O)	(segid 3A4 and resid 277 and name O)	3.42	0.04	0.04
	assign (segid 3A4 and resid 276 and name O)	(segid 3A4 and resid 278 and name C)	4.07	0.10	0.09
	assign (segid 3A4 and resid 276 and name O)	(segid 3A4 and resid 278 and name CA)	4.31	0.08	0.08
	assign (segid 3A4 and resid 276 and name O)	(segid 3A4 and resid 278 and name CB)	5.25	0.09	0.10
	assign (segid 3A4 and resid 276 and name O)	(segid 3A4 and resid 278 and name N)	3.36	0.09	0.09
30	assign (segid 3A4 and resid 276 and name O)	(segid 3A4 and resid 278 and name O)	4.98	0.11	0.12
	assign (segid 3A4 and resid 276 and name O)	(segid 3A4 and resid 279 and name C)	3.84	0.12	0.11
	assign (segid 3A4 and resid 276 and name O)	(segid 3A4 and resid 279 and name CA)	3.73	0.07	0.08
	assign (segid 3A4 and resid 276 and name O)	(segid 3A4 and resid 279 and name CB)	3.53	0.16	0.16
	assign (segid 3A4 and resid 276 and name O)	(segid 3A4 and resid 279 and name N)	3.28	0.05	0.05
35	assign (segid 3A4 and resid 276 and name O)	(segid 3A4 and resid 279 and name O)	5.02	0.12	0.12
	assign (segid 3A4 and resid 276 and name O)	(segid 3A4 and resid 280 and name C)	5.09	0.19	0.19
	assign (segid 3A4 and resid 276 and name O)	(segid 3A4 and resid 280 and name CA)	3.95	0.17	0.16
	assign (segid 3A4 and resid 276 and name O)	(segid 3A4 and resid 280 and name CB)	3.69	0.18	0.18
	assign (segid 3A4 and resid 276 and name O)	(segid 3A4 and resid 280 and name N)	3.04	0.15	0.14
40	assign (segid 3A4 and resid 276 and name O)	(segid 3A4 and resid 280 and name O)	6.23	0.18	0.18
	assign (segid 3A4 and resid 276 and name O)	(segid 3A4 and resid 281 and name C)	7.30	0.18	0.17
	assign (segid 3A4 and resid 276 and name O)	(segid 3A4 and resid 281 and name CA)	6.44	0.18	0.18
	assign (segid 3A4 and resid 276 and name O)	(segid 3A4 and resid 281 and name CB)	6.64	0.14	0.15
	assign (segid 3A4 and resid 276 and name O)	(segid 3A4 and resid 281 and name N)	5.08	0.18	0.17
45	assign (segid 3A4 and resid 276 and name O)	(segid 3A4 and resid 282 and name N)	6.93	0.18	0.19
	assign (segid 3A4 and resid 276 and name O)	(segid 3A4 and resid 308 and name CB)	6.73	0.26	0.26
	assign (segid 3A4 and resid 276 and name O)	(segid 3A4 and resid 365 and name CB)	6.45	0.72	0.73
	assign (segid 3A4 and resid 277 and name C)	(segid 3A4 and resid 277 and name CB)	2.48	0.03	0.03
50	assign (segid 3A4 and resid 277 and name C)	(segid 3A4 and resid 277 and name O)	1.24	0.02	0.01
	assign (segid 3A4 and resid 277 and name C)	(segid 3A4 and resid 278 and name C)	3.04	0.03	0.03
	assign (segid 3A4 and resid 277 and name C)	(segid 3A4 and resid 278 and name CA)	2.44	0.02	0.02
	assign (segid 3A4 and resid 277 and name C)	(segid 3A4 and resid 278 and name CB)	3.71	0.06	0.05
	assign (segid 3A4 and resid 277 and name C)	(segid 3A4 and resid 278 and name N)	1.33	0.01	0.01
	assign (segid 3A4 and resid 277 and name C)	(segid 3A4 and resid 278 and name O)	3.86	0.06	0.06
55	assign (segid 3A4 and resid 277 and name C)	(segid 3A4 and resid 279 and name C)	4.54	0.04	0.04
	assign (segid 3A4 and resid 277 and name C)	(segid 3A4 and resid 279 and name CA)	4.47	0.06	0.07
	assign (segid 3A4 and resid 277 and name C)	(segid 3A4 and resid 279 and name CB)	5.15	0.14	0.13
	assign (segid 3A4 and resid 277 and name C)	(segid 3A4 and resid 279 and name N)	3.32	0.07	0.07
	assign (segid 3A4 and resid 277 and name C)	(segid 3A4 and resid 279 and name O)	5.61	0.07	0.07
60	assign (segid 3A4 and resid 277 and name C)	(segid 3A4 and resid 280 and name C)	4.84	0.08	0.08
	assign (segid 3A4 and resid 277 and name C)	(segid 3A4 and resid 280 and name CA)	4.52	0.03	0.04
	assign (segid 3A4 and resid 277 and name C)	(segid 3A4 and resid 280 and name CB)	4.35	0.10	0.11
	assign (segid 3A4 and resid 277 and name C)	(segid 3A4 and resid 280 and name N)	3.80	0.05	0.04
	assign (segid 3A4 and resid 277 and name C)	(segid 3A4 and resid 280 and name O)	6.04	0.07	0.07
65	assign (segid 3A4 and resid 277 and name C)	(segid 3A4 and resid 281 and name C)	6.07	0.13	0.12
	assign (segid 3A4 and resid 277 and name C)	(segid 3A4 and resid 281 and name CA)	4.99	0.11	0.10
	assign (segid 3A4 and resid 277 and name C)	(segid 3A4 and resid 281 and name CB)	4.57	0.09	0.09
	assign (segid 3A4 and resid 277 and name C)	(segid 3A4 and resid 281 and name N)	4.08	0.09	0.10
	assign (segid 3A4 and resid 277 and name C)	(segid 3A4 and resid 281 and name O)	7.23	0.14	0.13
70	assign (segid 3A4 and resid 277 and name C)	(segid 3A4 and resid 282 and name CA)	7.23	0.15	0.15
	assign (segid 3A4 and resid 277 and name C)	(segid 3A4 and resid 282 and name N)	5.95	0.13	0.12
	assign (segid 3A4 and resid 277 and name C)	(segid 3A4 and resid 409 and name CB)	6.73	0.36	0.36
	assign (segid 3A4 and resid 277 and name C)	(segid 3A4 and resid 409 and name CD2)	6.07	0.63	0.63
	assign (segid 3A4 and resid 277 and name C)	(segid 3A4 and resid 409 and name CG)	6.42	0.48	0.48
75	assign (segid 3A4 and resid 277 and name CA)	(segid 3A4 and resid 277 and name C)	1.51	0.01	0.02
	assign (segid 3A4 and resid 277 and name CA)	(segid 3A4 and resid 277 and name CB)	1.53	0.01	0.00
	assign (segid 3A4 and resid 277 and name CA)	(segid 3A4 and resid 277 and name O)	2.40	0.02	0.02
	assign (segid 3A4 and resid 277 and name CA)	(segid 3A4 and resid 278 and name C)	4.42	0.03	0.03
	assign (segid 3A4 and resid 277 and name CA)	(segid 3A4 and resid 278 and name CA)	3.79	0.02	0.02
80	assign (segid 3A4 and resid 277 and name CA)	(segid 3A4 and resid 278 and name CB)	4.83	0.05	0.05
	assign (segid 3A4 and resid 277 and name CA)	(segid 3A4 and resid 278 and name N)	2.41	0.02	0.02
	assign (segid 3A4 and resid 277 and name CA)	(segid 3A4 and resid 278 and name O)	5.32	0.06	0.06
	assign (segid 3A4 and resid 277 and name CA)	(segid 3A4 and resid 279 and name C)	5.52	0.06	0.07

	assign (segid 3A4 and resid 277 and name CA) (segid 3A4 and resid 279 and name CA)	5.48	0.07	0.07
	assign (segid 3A4 and resid 277 and name CA) (segid 3A4 and resid 279 and name CB)	5.81	0.16	0.17
	assign (segid 3A4 and resid 277 and name CA) (segid 3A4 and resid 279 and name N)	4.42	0.06	0.06
	assign (segid 3A4 and resid 277 and name CA) (segid 3A4 and resid 279 and name O)	6.65	0.09	0.08
	assign (segid 3A4 and resid 277 and name CA) (segid 3A4 and resid 280 and name C)	5.73	0.14	0.13
5	assign (segid 3A4 and resid 277 and name CA) (segid 3A4 and resid 280 and name CA)	5.17	0.11	0.11
	assign (segid 3A4 and resid 277 and name CA) (segid 3A4 and resid 280 and name CB)	4.58	0.19	0.19
	assign (segid 3A4 and resid 277 and name CA) (segid 3A4 and resid 280 and name N)	4.58	0.06	0.07
	assign (segid 3A4 and resid 277 and name CA) (segid 3A4 and resid 280 and name O)	6.90	0.12	0.12
	assign (segid 3A4 and resid 277 and name CA) (segid 3A4 and resid 281 and name C)	7.35	0.16	0.16
10	assign (segid 3A4 and resid 277 and name CA) (segid 3A4 and resid 281 and name CA)	6.16	0.16	0.16
	assign (segid 3A4 and resid 277 and name CA) (segid 3A4 and resid 281 and name CB)	5.81	0.14	0.13
	assign (segid 3A4 and resid 277 and name CA) (segid 3A4 and resid 281 and name N)	5.17	0.14	0.14
	assign (segid 3A4 and resid 277 and name CA) (segid 3A4 and resid 282 and name CA)	8.62	0.16	0.17
	assign (segid 3A4 and resid 277 and name CA) (segid 3A4 and resid 282 and name N)	7.32	0.16	0.15
15	assign (segid 3A4 and resid 277 and name CA) (segid 3A4 and resid 303 and name CA)	13.22	0.37	0.37
	assign (segid 3A4 and resid 277 and name CA) (segid 3A4 and resid 303 and name CB)	14.14	0.33	0.33
	assign (segid 3A4 and resid 277 and name CA) (segid 3A4 and resid 304 and name CA)	10.48	0.30	0.30
	assign (segid 3A4 and resid 277 and name CA) (segid 3A4 and resid 304 and name CB)	9.52	0.35	0.36
20	assign (segid 3A4 and resid 277 and name CA) (segid 3A4 and resid 305 and name CA)	9.85	0.46	0.45
	assign (segid 3A4 and resid 277 and name CA) (segid 3A4 and resid 305 and name CB)	10.20	0.50	0.49
	assign (segid 3A4 and resid 277 and name CA) (segid 3A4 and resid 306 and name CA)	13.17	0.45	0.46
	assign (segid 3A4 and resid 277 and name CA) (segid 3A4 and resid 307 and name CA)	12.51	0.43	0.44
	assign (segid 3A4 and resid 277 and name CA) (segid 3A4 and resid 307 and name CB)	12.32	0.50	0.51
25	assign (segid 3A4 and resid 277 and name CA) (segid 3A4 and resid 308 and name CA)	9.54	0.35	0.35
	assign (segid 3A4 and resid 277 and name CA) (segid 3A4 and resid 308 and name CB)	8.25	0.38	0.38
	assign (segid 3A4 and resid 277 and name CA) (segid 3A4 and resid 309 and name CA)	12.09	0.49	0.49
	assign (segid 3A4 and resid 277 and name CA) (segid 3A4 and resid 309 and name CB)	12.88	0.56	0.55
	assign (segid 3A4 and resid 277 and name CA) (segid 3A4 and resid 310 and name CA)	14.73	0.39	0.38
	assign (segid 3A4 and resid 277 and name CA) (segid 3A4 and resid 310 and name CB)	15.31	0.43	0.42
30	assign (segid 3A4 and resid 277 and name CA) (segid 3A4 and resid 311 and name CA)	13.14	0.31	0.31
	assign (segid 3A4 and resid 277 and name CA) (segid 3A4 and resid 311 and name CB)	12.09	0.34	0.33
	assign (segid 3A4 and resid 277 and name CA) (segid 3A4 and resid 312 and name CA)	12.52	0.33	0.34
	assign (segid 3A4 and resid 277 and name CA) (segid 3A4 and resid 312 and name CB)	11.82	0.38	0.39
35	assign (segid 3A4 and resid 277 and name CA) (segid 3A4 and resid 313 and name CA)	16.17	0.34	0.34
	assign (segid 3A4 and resid 277 and name CA) (segid 3A4 and resid 313 and name CB)	16.81	0.34	0.34
	assign (segid 3A4 and resid 277 and name CA) (segid 3A4 and resid 314 and name CA)	17.32	0.30	0.30
	assign (segid 3A4 and resid 277 and name CA) (segid 3A4 and resid 314 and name CB)	17.06	0.29	0.29
	assign (segid 3A4 and resid 277 and name CA) (segid 3A4 and resid 315 and name CA)	15.92	0.48	0.48
	assign (segid 3A4 and resid 277 and name CA) (segid 3A4 and resid 315 and name CB)	14.54	0.53	0.53
40	assign (segid 3A4 and resid 277 and name CA) (segid 3A4 and resid 316 and name CA)	16.90	0.50	0.51
	assign (segid 3A4 and resid 277 and name CA) (segid 3A4 and resid 316 and name CB)	18.00	0.58	0.58
	assign (segid 3A4 and resid 277 and name CA) (segid 3A4 and resid 362 and name CA)	14.92	0.55	0.54
	assign (segid 3A4 and resid 277 and name CA) (segid 3A4 and resid 362 and name CB)	15.18	0.59	0.59
	assign (segid 3A4 and resid 277 and name CA) (segid 3A4 and resid 363 and name CA)	11.72	0.45	0.45
45	assign (segid 3A4 and resid 277 and name CA) (segid 3A4 and resid 363 and name CB)	10.78	0.43	0.43
	assign (segid 3A4 and resid 277 and name CA) (segid 3A4 and resid 364 and name CA)	11.25	0.59	0.59
	assign (segid 3A4 and resid 277 and name CA) (segid 3A4 and resid 364 and name CB)	12.49	0.63	0.62
	assign (segid 3A4 and resid 277 and name CA) (segid 3A4 and resid 365 and name CA)	10.13	0.69	0.68
	assign (segid 3A4 and resid 277 and name CA) (segid 3A4 and resid 365 and name CB)	8.82	0.73	0.72
50	assign (segid 3A4 and resid 277 and name CA) (segid 3A4 and resid 398 and name CA)	18.30	0.25	0.24
	assign (segid 3A4 and resid 277 and name CA) (segid 3A4 and resid 398 and name CB)	18.73	0.27	0.28
	assign (segid 3A4 and resid 277 and name CA) (segid 3A4 and resid 399 and name CA)	18.89	0.31	0.31
	assign (segid 3A4 and resid 277 and name CA) (segid 3A4 and resid 400 and name CA)	18.19	0.42	0.42
	assign (segid 3A4 and resid 277 and name CA) (segid 3A4 and resid 400 and name CB)	19.06	0.46	0.46
55	assign (segid 3A4 and resid 277 and name CA) (segid 3A4 and resid 401 and name CA)	14.89	0.38	0.38
	assign (segid 3A4 and resid 277 and name CA) (segid 3A4 and resid 402 and name CA)	13.74	0.34	0.34
	assign (segid 3A4 and resid 277 and name CA) (segid 3A4 and resid 402 and name CB)	14.60	0.34	0.34
	assign (segid 3A4 and resid 277 and name CA) (segid 3A4 and resid 403 and name CA)	15.27	0.39	0.39
	assign (segid 3A4 and resid 277 and name CA) (segid 3A4 and resid 403 and name CB)	16.77	0.38	0.38
60	assign (segid 3A4 and resid 277 and name CA) (segid 3A4 and resid 404 and name CA)	13.91	0.52	0.53
	assign (segid 3A4 and resid 277 and name CA) (segid 3A4 and resid 404 and name CB)	14.27	0.61	0.62
	assign (segid 3A4 and resid 277 and name CA) (segid 3A4 and resid 405 and name CA)	10.27	0.45	0.44
	assign (segid 3A4 and resid 277 and name CA) (segid 3A4 and resid 405 and name CB)	9.74	0.35	0.35
	assign (segid 3A4 and resid 277 and name CA) (segid 3A4 and resid 406 and name CA)	10.84	0.54	0.53
65	assign (segid 3A4 and resid 277 and name CA) (segid 3A4 and resid 407 and name CA)	12.83	0.43	0.43
	assign (segid 3A4 and resid 277 and name CA) (segid 3A4 and resid 407 and name CB)	14.20	0.37	0.37
	assign (segid 3A4 and resid 277 and name CA) (segid 3A4 and resid 408 and name CA)	11.06	0.39	0.39
	assign (segid 3A4 and resid 277 and name CA) (segid 3A4 and resid 408 and name CB)	10.70	0.37	0.37
70	assign (segid 3A4 and resid 277 and name CA) (segid 3A4 and resid 409 and name CA)	8.01	0.49	0.49
	assign (segid 3A4 and resid 277 and name CA) (segid 3A4 and resid 409 and name CB)	6.85	0.39	0.39
	assign (segid 3A4 and resid 277 and name CA) (segid 3A4 and resid 409 and name CB2)	5.73	0.65	0.64
	assign (segid 3A4 and resid 277 and name CA) (segid 3A4 and resid 409 and name CG)	6.23	0.51	0.50
	assign (segid 3A4 and resid 277 and name CA) (segid 3A4 and resid 410 and name CA)	10.63	0.48	0.49
	assign (segid 3A4 and resid 277 and name CA) (segid 3A4 and resid 411 and name CA)	12.75	0.70	0.70
75	assign (segid 3A4 and resid 277 and name CA) (segid 3A4 and resid 411 and name CB)	13.64	0.63	0.62
	assign (segid 3A4 and resid 277 and name CA) (segid 3A4 and resid 412 and name CA)	10.95	0.97	0.96
	assign (segid 3A4 and resid 277 and name CA) (segid 3A4 and resid 413 and name CA)	9.67	1.06	1.06
	assign (segid 3A4 and resid 277 and name CA) (segid 3A4 and resid 414 and name CA)	9.83	0.91	0.91
80	assign (segid 3A4 and resid 277 and name CA) (segid 3A4 and resid 415 and name CA)	11.46	0.94	0.94
	assign (segid 3A4 and resid 277 and name CA) (segid 3A4 and resid 415 and name CB)	12.13	0.88	0.88
	assign (segid 3A4 and resid 277 and name CA) (segid 3A4 and resid 416 and name CA)	13.67	1.37	1.36
	assign (segid 3A4 and resid 277 and name CA) (segid 3A4 and resid 417 and name CA)	16.93	0.95	0.96

5	assign	(segid 3A4 and resid 277 and name CA)	(segid 3A4 and resid 438 and name CA)	17.08	0.19	0.19
	assign	(segid 3A4 and resid 277 and name CA)	(segid 3A4 and resid 439 and name CA)	17.40	0.33	0.33
	assign	(segid 3A4 and resid 277 and name CA)	(segid 3A4 and resid 440 and name CA)	14.67	0.33	0.34
	assign	(segid 3A4 and resid 277 and name CB)	(segid 3A4 and resid 278 and name C)	5.41	0.03	0.03
10	assign	(segid 3A4 and resid 277 and name CB)	(segid 3A4 and resid 278 and name CA)	4.43	0.06	0.05
	assign	(segid 3A4 and resid 277 and name CB)	(segid 3A4 and resid 278 and name CB)	5.27	0.08	0.09
	assign	(segid 3A4 and resid 277 and name CB)	(segid 3A4 and resid 278 and name N)	3.12	0.06	0.05
	assign	(segid 3A4 and resid 277 and name CB)	(segid 3A4 and resid 278 and name O)	6.26	0.05	0.06
15	assign	(segid 3A4 and resid 277 and name CB)	(segid 3A4 and resid 279 and name C)	6.91	0.05	0.05
	assign	(segid 3A4 and resid 277 and name CB)	(segid 3A4 and resid 279 and name CA)	6.82	0.07	0.06
	assign	(segid 3A4 and resid 277 and name CB)	(segid 3A4 and resid 279 and name CB)	7.22	0.16	0.16
	assign	(segid 3A4 and resid 277 and name CB)	(segid 3A4 and resid 279 and name N)	5.63	0.07	0.06
20	assign	(segid 3A4 and resid 277 and name CB)	(segid 3A4 and resid 280 and name C)	6.85	0.11	0.12
	assign	(segid 3A4 and resid 277 and name CB)	(segid 3A4 and resid 280 and name CA)	6.49	0.09	0.10
	assign	(segid 3A4 and resid 277 and name CB)	(segid 3A4 and resid 280 and name CB)	5.83	0.21	0.20
	assign	(segid 3A4 and resid 277 and name CB)	(segid 3A4 and resid 280 and name N)	6.00	0.05	0.05
25	assign	(segid 3A4 and resid 277 and name CB)	(segid 3A4 and resid 281 and name CA)	6.88	0.14	0.15
	assign	(segid 3A4 and resid 277 and name CB)	(segid 3A4 and resid 281 and name CB)	6.25	0.14	0.14
	assign	(segid 3A4 and resid 277 and name CB)	(segid 3A4 and resid 281 and name N)	6.13	0.12	0.13
	assign	(segid 3A4 and resid 277 and name CB)	(segid 3A4 and resid 282 and name CA)	9.58	0.15	0.14
30	assign	(segid 3A4 and resid 277 and name CB)	(segid 3A4 and resid 303 and name CA)	14.55	0.41	0.42
	assign	(segid 3A4 and resid 277 and name CB)	(segid 3A4 and resid 303 and name CB)	15.51	0.36	0.36
	assign	(segid 3A4 and resid 277 and name CB)	(segid 3A4 and resid 304 and name CA)	11.91	0.31	0.31
	assign	(segid 3A4 and resid 277 and name CB)	(segid 3A4 and resid 304 and name CB)	10.99	0.35	0.36
35	assign	(segid 3A4 and resid 277 and name CB)	(segid 3A4 and resid 305 and name CA)	11.03	0.45	0.45
	assign	(segid 3A4 and resid 277 and name CB)	(segid 3A4 and resid 305 and name CB)	11.28	0.47	0.47
	assign	(segid 3A4 and resid 277 and name CB)	(segid 3A4 and resid 306 and name CA)	14.34	0.48	0.49
	assign	(segid 3A4 and resid 277 and name CB)	(segid 3A4 and resid 307 and name CA)	13.79	0.48	0.49
40	assign	(segid 3A4 and resid 277 and name CB)	(segid 3A4 and resid 307 and name CB)	13.69	0.54	0.53
	assign	(segid 3A4 and resid 277 and name CB)	(segid 3A4 and resid 308 and name CA)	10.65	0.44	0.44
	assign	(segid 3A4 and resid 277 and name CB)	(segid 3A4 and resid 308 and name CB)	9.35	0.46	0.46
	assign	(segid 3A4 and resid 277 and name CB)	(segid 3A4 and resid 309 and name CA)	12.93	0.56	0.56
45	assign	(segid 3A4 and resid 277 and name CB)	(segid 3A4 and resid 309 and name CB)	13.72	0.62	0.62
	assign	(segid 3A4 and resid 277 and name CB)	(segid 3A4 and resid 310 and name CA)	15.69	0.47	0.47
	assign	(segid 3A4 and resid 277 and name CB)	(segid 3A4 and resid 310 and name CB)	16.37	0.50	0.50
	assign	(segid 3A4 and resid 277 and name CB)	(segid 3A4 and resid 311 and name CA)	14.04	0.38	0.38
50	assign	(segid 3A4 and resid 277 and name CB)	(segid 3A4 and resid 311 and name CB)	13.04	0.40	0.41
	assign	(segid 3A4 and resid 277 and name CB)	(segid 3A4 and resid 312 and name CA)	13.07	0.38	0.38
	assign	(segid 3A4 and resid 277 and name CB)	(segid 3A4 and resid 312 and name CB)	12.31	0.41	0.42
	assign	(segid 3A4 and resid 277 and name CB)	(segid 3A4 and resid 313 and name CA)	16.73	0.40	0.40
55	assign	(segid 3A4 and resid 277 and name CB)	(segid 3A4 and resid 313 and name CB)	17.44	0.40	0.41
	assign	(segid 3A4 and resid 277 and name CB)	(segid 3A4 and resid 314 and name CA)	17.98	0.34	0.35
	assign	(segid 3A4 and resid 277 and name CB)	(segid 3A4 and resid 314 and name CB)	17.82	0.35	0.36
	assign	(segid 3A4 and resid 277 and name CB)	(segid 3A4 and resid 315 and name CA)	16.36	0.46	0.46
60	assign	(segid 3A4 and resid 277 and name CB)	(segid 3A4 and resid 315 and name CB)	14.97	0.51	0.50
	assign	(segid 3A4 and resid 277 and name CB)	(segid 3A4 and resid 316 and name CA)	17.10	0.48	0.47
	assign	(segid 3A4 and resid 277 and name CB)	(segid 3A4 and resid 361 and name CA)	18.38	0.56	0.55
	assign	(segid 3A4 and resid 277 and name CB)	(segid 3A4 and resid 362 and name CA)	15.40	0.54	0.54
65	assign	(segid 3A4 and resid 277 and name CB)	(segid 3A4 and resid 362 and name CB)	15.73	0.60	0.60
	assign	(segid 3A4 and resid 277 and name CB)	(segid 3A4 and resid 363 and name CA)	12.29	0.46	0.47
	assign	(segid 3A4 and resid 277 and name CB)	(segid 3A4 and resid 363 and name CB)	11.23	0.45	0.44
	assign	(segid 3A4 and resid 277 and name CB)	(segid 3A4 and resid 364 and name CA)	12.21	0.61	0.60
70	assign	(segid 3A4 and resid 277 and name CB)	(segid 3A4 and resid 364 and name CB)	13.46	0.64	0.63
	assign	(segid 3A4 and resid 277 and name CB)	(segid 3A4 and resid 365 and name CA)	11.36	0.68	0.67
	assign	(segid 3A4 and resid 277 and name CB)	(segid 3A4 and resid 365 and name CB)	10.10	0.72	0.72
	assign	(segid 3A4 and resid 277 and name CB)	(segid 3A4 and resid 398 and name CA)	18.99	0.28	0.28
75	assign	(segid 3A4 and resid 277 and name CB)	(segid 3A4 and resid 398 and name CB)	19.53	0.27	0.27
	assign	(segid 3A4 and resid 277 and name CB)	(segid 3A4 and resid 400 and name CA)	18.56	0.51	0.51
	assign	(segid 3A4 and resid 277 and name CB)	(segid 3A4 and resid 401 and name CA)	15.30	0.44	0.44
	assign	(segid 3A4 and resid 277 and name CB)	(segid 3A4 and resid 402 and name CA)	14.40	0.41	0.42
80	assign	(segid 3A4 and resid 277 and name CB)	(segid 3A4 and resid 402 and name CB)	15.38	0.41	0.41
	assign	(segid 3A4 and resid 277 and name CB)	(segid 3A4 and resid 403 and name CA)	15.72	0.47	0.46
	assign	(segid 3A4 and resid 277 and name CB)	(segid 3A4 and resid 403 and name CB)	17.18	0.46	0.46
	assign	(segid 3A4 and resid 277 and name CB)	(segid 3A4 and resid 404 and name CA)	14.03	0.55	0.56
85	assign	(segid 3A4 and resid 277 and name CB)	(segid 3A4 and resid 404 and name CB)	14.33	0.62	0.63
	assign	(segid 3A4 and resid 277 and name CB)	(segid 3A4 and resid 405 and name CA)	10.51	0.47	0.46
	assign	(segid 3A4 and resid 277 and name CB)	(segid 3A4 and resid 405 and name CB)	10.11	0.37	0.37
	assign	(segid 3A4 and resid 277 and name CB)	(segid 3A4 and resid 406 and name CA)	11.30	0.62	0.62
90	assign	(segid 3A4 and resid 277 and name CB)	(segid 3A4 and resid 407 and name CA)	12.91	0.48	0.47
	assign	(segid 3A4 and resid 277 and name CB)	(segid 3A4 and resid 407 and name CB)	14.24	0.41	0.42
	assign	(segid 3A4 and resid 277 and name CB)	(segid 3A4 and resid 408 and name CA)	10.74	0.42	0.43
	assign	(segid 3A4 and resid 277 and name CB)	(segid 3A4 and resid 408 and name CB)	10.33	0.38	0.38
95	assign	(segid 3A4 and resid 277 and name CB)	(segid 3A4 and resid 409 and name CA)	7.79	0.50	0.49
	assign	(segid 3A4 and resid 277 and name CB)	(segid 3A4 and resid 409 and name CB)	6.82	0.43	0.43
	assign	(segid 3A4 and resid 277 and name CB)	(segid 3A4 and resid 409 and name CG2)	5.33	0.65	0.65
	assign	(segid 3A4 and resid 277 and name CB)	(segid 3A4 and resid 409 and name CD)	6.14	0.55	0.55
100	assign	(segid 3A4 and resid 277 and name CB)	(segid 3A4 and resid 410 and name CA)	10.58	0.57	0.57
	assign	(segid 3A4 and resid 277 and name CB)	(segid 3A4 and resid 411 and name CA)	12.29	0.79	0.79
	assign	(segid 3A4 and resid 277 and name CB)	(segid 3A4 and resid 411 and name CB)	13.16	0.72	0.72
	assign	(segid 3A4 and resid 277 and name CB)	(segid 3A4 and resid 412 and name CA)	10.11	1.05	1.04
105	assign	(segid 3A4 and resid 277 and name CB)	(segid 3A4 and resid 413 and name CA)	8.47	1.11	1.11
	assign	(segid 3A4 and resid 277 and name CB)	(segid 3A4 and resid 414 and name CA)	8.49	0.95	0.95
	assign	(segid 3A4 and resid 277 and name CB)	(segid 3A4 and resid 415 and name CA)	10.05	1.01	1.01

	assign (segid 3A4 and resid 277 and name CB)	(segid 3A4 and resid 415 and name CB)	10.73	0.98	0.98
	assign (segid 3A4 and resid 277 and name CB)	(segid 3A4 and resid 416 and name CA)	12.29	1.41	1.40
	assign (segid 3A4 and resid 277 and name CB)	(segid 3A4 and resid 417 and name CA)	15.52	1.01	1.00
	assign (segid 3A4 and resid 277 and name CB)	(segid 3A4 and resid 423 and name CA)	18.02	1.24	1.24
5	assign (segid 3A4 and resid 277 and name CB)	(segid 3A4 and resid 435 and name CA)	18.48	0.60	0.61
	assign (segid 3A4 and resid 277 and name CB)	(segid 3A4 and resid 438 and name CA)	16.04	0.19	0.19
	assign (segid 3A4 and resid 277 and name CB)	(segid 3A4 and resid 439 and name CA)	16.16	0.34	0.35
	assign (segid 3A4 and resid 277 and name CB)	(segid 3A4 and resid 440 and name CA)	13.35	0.33	0.34
	assign (segid 3A4 and resid 277 and name N)	(segid 3A4 and resid 277 and name C)	2.45	0.02	0.02
	assign (segid 3A4 and resid 277 and name N)	(segid 3A4 and resid 277 and name CA)	1.46	0.01	0.01
10	assign (segid 3A4 and resid 277 and name N)	(segid 3A4 and resid 277 and name CB)	2.45	0.03	0.03
	assign (segid 3A4 and resid 277 and name N)	(segid 3A4 and resid 277 and name O)	3.50	0.02	0.03
	assign (segid 3A4 and resid 277 and name N)	(segid 3A4 and resid 278 and name C)	4.72	0.05	0.05
	assign (segid 3A4 and resid 277 and name N)	(segid 3A4 and resid 278 and name CA)	4.19	0.05	0.04
	assign (segid 3A4 and resid 277 and name N)	(segid 3A4 and resid 278 and name CB)	4.92	0.06	0.05
15	assign (segid 3A4 and resid 277 and name N)	(segid 3A4 and resid 278 and name N)	2.78	0.04	0.04
	assign (segid 3A4 and resid 277 and name N)	(segid 3A4 and resid 278 and name O)	5.79	0.05	0.06
	assign (segid 3A4 and resid 277 and name N)	(segid 3A4 and resid 279 and name C)	5.67	0.08	0.07
	assign (segid 3A4 and resid 277 and name N)	(segid 3A4 and resid 279 and name CA)	5.34	0.09	0.10
	assign (segid 3A4 and resid 277 and name N)	(segid 3A4 and resid 279 and name CB)	5.32	0.20	0.20
20	assign (segid 3A4 and resid 277 and name N)	(segid 3A4 and resid 279 and name N)	4.35	0.08	0.08
	assign (segid 3A4 and resid 277 and name N)	(segid 3A4 and resid 279 and name O)	6.87	0.08	0.08
	assign (segid 3A4 and resid 277 and name N)	(segid 3A4 and resid 280 and name C)	6.50	0.15	0.14
	assign (segid 3A4 and resid 277 and name N)	(segid 3A4 and resid 280 and name CA)	5.67	0.13	0.13
	assign (segid 3A4 and resid 277 and name N)	(segid 3A4 and resid 280 and name CB)	5.16	0.21	0.20
25	assign (segid 3A4 and resid 277 and name N)	(segid 3A4 and resid 280 and name N)	4.86	0.08	0.08
	assign (segid 3A4 and resid 277 and name N)	(segid 3A4 and resid 280 and name O)	7.70	0.14	0.13
	assign (segid 3A4 and resid 277 and name N)	(segid 3A4 and resid 281 and name CA)	7.23	0.14	0.14
	assign (segid 3A4 and resid 277 and name N)	(segid 3A4 and resid 281 and name CB)	6.98	0.12	0.11
	assign (segid 3A4 and resid 277 and name N)	(segid 3A4 and resid 281 and name N)	6.11	0.14	0.13
30	assign (segid 3A4 and resid 277 and name N)	(segid 3A4 and resid 277 and name CB)	3.30	0.06	0.05
	assign (segid 3A4 and resid 277 and name O)	(segid 3A4 and resid 278 and name C)	2.99	0.06	0.06
	assign (segid 3A4 and resid 277 and name O)	(segid 3A4 and resid 278 and name CA)	2.78	0.05	0.04
	assign (segid 3A4 and resid 277 and name O)	(segid 3A4 and resid 278 and name CB)	4.25	0.06	0.06
	assign (segid 3A4 and resid 277 and name O)	(segid 3A4 and resid 278 and name N)	2.25	0.02	0.02
35	assign (segid 3A4 and resid 277 and name O)	(segid 3A4 and resid 278 and name O)	3.45	0.08	0.07
	assign (segid 3A4 and resid 277 and name O)	(segid 3A4 and resid 279 and name C)	4.10	0.10	0.11
	assign (segid 3A4 and resid 277 and name O)	(segid 3A4 and resid 279 and name CA)	4.40	0.11	0.12
	assign (segid 3A4 and resid 277 and name O)	(segid 3A4 and resid 279 and name CB)	5.30	0.18	0.19
	assign (segid 3A4 and resid 277 and name O)	(segid 3A4 and resid 279 and name N)	3.48	0.12	0.12
40	assign (segid 3A4 and resid 277 and name O)	(segid 3A4 and resid 279 and name O)	5.01	0.10	0.10
	assign (segid 3A4 and resid 277 and name O)	(segid 3A4 and resid 280 and name C)	3.78	0.09	0.09
	assign (segid 3A4 and resid 277 and name O)	(segid 3A4 and resid 280 and name CA)	3.73	0.10	0.10
	assign (segid 3A4 and resid 277 and name O)	(segid 3A4 and resid 280 and name CB)	3.65	0.08	0.09
	assign (segid 3A4 and resid 277 and name O)	(segid 3A4 and resid 280 and name N)	3.28	0.14	0.13
45	assign (segid 3A4 and resid 277 and name O)	(segid 3A4 and resid 280 and name O)	4.94	0.08	0.09
	assign (segid 3A4 and resid 277 and name O)	(segid 3A4 and resid 281 and name C)	4.98	0.15	0.15
	assign (segid 3A4 and resid 277 and name O)	(segid 3A4 and resid 281 and name CA)	3.92	0.13	0.12
	assign (segid 3A4 and resid 277 and name O)	(segid 3A4 and resid 281 and name CB)	3.52	0.13	0.12
	assign (segid 3A4 and resid 277 and name O)	(segid 3A4 and resid 281 and name N)	2.94	0.11	0.10
50	assign (segid 3A4 and resid 277 and name O)	(segid 3A4 and resid 281 and name O)	6.10	0.15	0.16
	assign (segid 3A4 and resid 277 and name O)	(segid 3A4 and resid 282 and name C)	7.20	0.13	0.14
	assign (segid 3A4 and resid 277 and name O)	(segid 3A4 and resid 282 and name CA)	6.37	0.18	0.19
	assign (segid 3A4 and resid 277 and name O)	(segid 3A4 and resid 282 and name N)	5.01	0.17	0.17
	assign (segid 3A4 and resid 277 and name O)	(segid 3A4 and resid 409 and name CA)	7.04	0.48	0.48
55	assign (segid 3A4 and resid 277 and name O)	(segid 3A4 and resid 409 and name CB)	5.86	0.38	0.38
	assign (segid 3A4 and resid 277 and name O)	(segid 3A4 and resid 409 and name CD2)	5.60	0.65	0.64
	assign (segid 3A4 and resid 277 and name O)	(segid 3A4 and resid 409 and name CG)	5.74	0.49	0.49
	assign (segid 3A4 and resid 277 and name O)	(segid 3A4 and resid 409 and name O)	6.98	0.57	0.57
	assign (segid 3A4 and resid 278 and name C)	(segid 3A4 and resid 278 and name CB)	2.48	0.03	0.02
60	assign (segid 3A4 and resid 278 and name C)	(segid 3A4 and resid 278 and name O)	1.23	0.00	0.00
	assign (segid 3A4 and resid 278 and name C)	(segid 3A4 and resid 279 and name C)	3.00	0.04	0.04
	assign (segid 3A4 and resid 278 and name C)	(segid 3A4 and resid 279 and name CA)	2.43	0.02	0.01
	assign (segid 3A4 and resid 278 and name C)	(segid 3A4 and resid 279 and name CB)	3.66	0.04	0.05
	assign (segid 3A4 and resid 278 and name C)	(segid 3A4 and resid 279 and name N)	1.33	0.00	0.00
65	assign (segid 3A4 and resid 278 and name C)	(segid 3A4 and resid 279 and name O)	3.84	0.07	0.07
	assign (segid 3A4 and resid 278 and name C)	(segid 3A4 and resid 280 and name C)	4.52	0.04	0.05
	assign (segid 3A4 and resid 278 and name C)	(segid 3A4 and resid 280 and name CA)	4.45	0.06	0.06
	assign (segid 3A4 and resid 278 and name C)	(segid 3A4 and resid 280 and name CB)	5.23	0.03	0.04
	assign (segid 3A4 and resid 278 and name C)	(segid 3A4 and resid 280 and name N)	3.27	0.07	0.07
70	assign (segid 3A4 and resid 278 and name C)	(segid 3A4 and resid 280 and name O)	5.61	0.04	0.03
	assign (segid 3A4 and resid 278 and name C)	(segid 3A4 and resid 281 and name C)	4.84	0.05	0.04
	assign (segid 3A4 and resid 278 and name C)	(segid 3A4 and resid 281 and name CA)	4.52	0.08	0.07
	assign (segid 3A4 and resid 278 and name C)	(segid 3A4 and resid 281 and name CB)	4.31	0.10	0.10
	assign (segid 3A4 and resid 278 and name C)	(segid 3A4 and resid 281 and name N)	3.79	0.08	0.07
75	assign (segid 3A4 and resid 278 and name C)	(segid 3A4 and resid 281 and name O)	6.04	0.04	0.04
	assign (segid 3A4 and resid 278 and name C)	(segid 3A4 and resid 282 and name C)	6.04	0.05	0.05
	assign (segid 3A4 and resid 278 and name C)	(segid 3A4 and resid 282 and name CA)	5.00	0.08	0.08
	assign (segid 3A4 and resid 278 and name C)	(segid 3A4 and resid 282 and name N)	4.10	0.05	0.05
	assign (segid 3A4 and resid 278 and name C)	(segid 3A4 and resid 282 and name O)	7.18	0.05	0.04
80	assign (segid 3A4 and resid 278 and name C)	(segid 3A4 and resid 282 and name O)	1.51	0.01	0.01
	assign (segid 3A4 and resid 278 and name CA)	(segid 3A4 and resid 278 and name C)	1.52	0.02	0.02
	assign (segid 3A4 and resid 278 and name CA)	(segid 3A4 and resid 278 and name CB)	2.39	0.01	0.02
	assign (segid 3A4 and resid 278 and name CA)	(segid 3A4 and resid 278 and name O)			

	assign (segid 3A4 and resid 278 and name CA)	(segid 3A4 and resid 279 and name C)	4.37	0.04	0.05
	assign (segid 3A4 and resid 278 and name CA)	(segid 3A4 and resid 279 and name CA)	3.78	0.02	0.02
	assign (segid 3A4 and resid 278 and name CA)	(segid 3A4 and resid 279 and name CB)	4.77	0.05	0.05
	assign (segid 3A4 and resid 278 and name CA)	(segid 3A4 and resid 279 and name N)	2.41	0.02	0.02
5	assign (segid 3A4 and resid 278 and name CA)	(segid 3A4 and resid 279 and name O)	5.29	0.08	0.08
	assign (segid 3A4 and resid 278 and name CA)	(segid 3A4 and resid 280 and name C)	5.45	0.06	0.06
	assign (segid 3A4 and resid 278 and name CA)	(segid 3A4 and resid 280 and name CA)	5.42	0.06	0.05
	assign (segid 3A4 and resid 278 and name CA)	(segid 3A4 and resid 280 and name CB)	5.88	0.05	0.05
	assign (segid 3A4 and resid 278 and name CA)	(segid 3A4 and resid 280 and name N)	4.34	0.06	0.06
	assign (segid 3A4 and resid 278 and name CA)	(segid 3A4 and resid 280 and name O)	6.58	0.06	0.07
10	assign (segid 3A4 and resid 278 and name CA)	(segid 3A4 and resid 281 and name C)	5.65	0.09	0.08
	assign (segid 3A4 and resid 278 and name CA)	(segid 3A4 and resid 281 and name CA)	5.07	0.07	0.08
	assign (segid 3A4 and resid 278 and name CA)	(segid 3A4 and resid 281 and name CB)	4.44	0.09	0.09
	assign (segid 3A4 and resid 278 and name CA)	(segid 3A4 and resid 281 and name N)	4.51	0.07	0.07
	assign (segid 3A4 and resid 278 and name CA)	(segid 3A4 and resid 281 and name O)	6.82	0.09	0.08
15	assign (segid 3A4 and resid 278 and name CA)	(segid 3A4 and resid 282 and name C)	7.29	0.06	0.06
	assign (segid 3A4 and resid 278 and name CA)	(segid 3A4 and resid 282 and name CA)	6.12	0.10	0.11
	assign (segid 3A4 and resid 278 and name CA)	(segid 3A4 and resid 282 and name N)	5.13	0.08	0.08
	assign (segid 3A4 and resid 278 and name CA)	(segid 3A4 and resid 303 and name CA)	13.27	0.59	0.59
20	assign (segid 3A4 and resid 278 and name CA)	(segid 3A4 and resid 303 and name CB)	13.88	0.53	0.54
	assign (segid 3A4 and resid 278 and name CA)	(segid 3A4 and resid 304 and name CA)	10.96	0.14	0.15
	assign (segid 3A4 and resid 278 and name CA)	(segid 3A4 and resid 304 and name CB)	9.73	0.19	0.19
	assign (segid 3A4 and resid 278 and name CA)	(segid 3A4 and resid 305 and name CA)	11.31	0.46	0.46
	assign (segid 3A4 and resid 278 and name CA)	(segid 3A4 and resid 305 and name CB)	11.60	0.58	0.59
25	assign (segid 3A4 and resid 278 and name CA)	(segid 3A4 and resid 306 and name CA)	14.87	0.37	0.38
	assign (segid 3A4 and resid 278 and name CA)	(segid 3A4 and resid 307 and name CA)	14.19	0.25	0.24
	assign (segid 3A4 and resid 278 and name CA)	(segid 3A4 and resid 307 and name CB)	13.66	0.34	0.34
	assign (segid 3A4 and resid 278 and name CA)	(segid 3A4 and resid 308 and name CA)	11.93	0.16	0.16
	assign (segid 3A4 and resid 278 and name CA)	(segid 3A4 and resid 308 and name CB)	10.66	0.23	0.24
	assign (segid 3A4 and resid 278 and name CA)	(segid 3A4 and resid 309 and name CA)	14.88	0.42	0.42
30	assign (segid 3A4 and resid 278 and name CA)	(segid 3A4 and resid 309 and name CB)	15.55	0.47	0.47
	assign (segid 3A4 and resid 278 and name CA)	(segid 3A4 and resid 310 and name CA)	17.30	0.26	0.27
	assign (segid 3A4 and resid 278 and name CA)	(segid 3A4 and resid 310 and name CB)	17.63	0.28	0.27
	assign (segid 3A4 and resid 278 and name CA)	(segid 3A4 and resid 311 and name CA)	15.84	0.23	0.23
	assign (segid 3A4 and resid 278 and name CA)	(segid 3A4 and resid 311 and name CB)	14.62	0.22	0.22
35	assign (segid 3A4 and resid 278 and name CA)	(segid 3A4 and resid 312 and name CA)	15.81	0.34	0.35
	assign (segid 3A4 and resid 278 and name CA)	(segid 3A4 and resid 312 and name CB)	15.21	0.41	0.40
	assign (segid 3A4 and resid 278 and name CA)	(segid 3A4 and resid 313 and name CA)	19.42	0.32	0.33
	assign (segid 3A4 and resid 278 and name CA)	(segid 3A4 and resid 315 and name CB)	17.70	0.57	0.57
	assign (segid 3A4 and resid 278 and name CA)	(segid 3A4 and resid 362 and name CA)	17.09	0.58	0.58
40	assign (segid 3A4 and resid 278 and name CA)	(segid 3A4 and resid 362 and name CB)	17.05	0.60	0.61
	assign (segid 3A4 and resid 278 and name CA)	(segid 3A4 and resid 363 and name CA)	14.22	0.44	0.45
	assign (segid 3A4 and resid 278 and name CA)	(segid 3A4 and resid 363 and name CB)	13.52	0.42	0.42
	assign (segid 3A4 and resid 278 and name CA)	(segid 3A4 and resid 364 and name CA)	13.01	0.52	0.51
	assign (segid 3A4 and resid 278 and name CA)	(segid 3A4 and resid 364 and name CB)	13.99	0.58	0.57
45	assign (segid 3A4 and resid 278 and name CA)	(segid 3A4 and resid 365 and name CA)	11.81	0.61	0.61
	assign (segid 3A4 and resid 278 and name CA)	(segid 3A4 and resid 365 and name CB)	10.49	0.63	0.62
	assign (segid 3A4 and resid 278 and name CA)	(segid 3A4 and resid 401 and name CA)	17.73	0.30	0.29
	assign (segid 3A4 and resid 278 and name CA)	(segid 3A4 and resid 402 and name CA)	15.96	0.31	0.31
	assign (segid 3A4 and resid 278 and name CA)	(segid 3A4 and resid 402 and name CB)	16.62	0.33	0.34
50	assign (segid 3A4 and resid 278 and name CA)	(segid 3A4 and resid 403 and name CA)	17.21	0.31	0.31
	assign (segid 3A4 and resid 278 and name CA)	(segid 3A4 and resid 403 and name CB)	18.72	0.32	0.31
	assign (segid 3A4 and resid 278 and name CA)	(segid 3A4 and resid 404 and name CA)	16.33	0.40	0.40
	assign (segid 3A4 and resid 278 and name CA)	(segid 3A4 and resid 404 and name CB)	16.95	0.47	0.47
	assign (segid 3A4 and resid 278 and name CA)	(segid 3A4 and resid 405 and name CA)	12.76	0.40	0.39
55	assign (segid 3A4 and resid 278 and name CA)	(segid 3A4 and resid 405 and name CB)	12.39	0.36	0.36
	assign (segid 3A4 and resid 278 and name CA)	(segid 3A4 and resid 406 and name CA)	12.29	0.43	0.44
	assign (segid 3A4 and resid 278 and name CA)	(segid 3A4 and resid 407 and name CA)	14.19	0.38	0.38
	assign (segid 3A4 and resid 278 and name CA)	(segid 3A4 and resid 407 and name CB)	15.67	0.34	0.34
	assign (segid 3A4 and resid 278 and name CA)	(segid 3A4 and resid 408 and name CA)	12.92	0.33	0.34
60	assign (segid 3A4 and resid 278 and name CA)	(segid 3A4 and resid 408 and name CB)	12.96	0.32	0.31
	assign (segid 3A4 and resid 278 and name CA)	(segid 3A4 and resid 409 and name CA)	9.32	0.40	0.40
	assign (segid 3A4 and resid 278 and name CA)	(segid 3A4 and resid 409 and name CB)	8.29	0.29	0.29
	assign (segid 3A4 and resid 278 and name CA)	(segid 3A4 and resid 410 and name CA)	10.80	0.44	0.45
	assign (segid 3A4 and resid 278 and name CA)	(segid 3A4 and resid 411 and name CA)	13.24	0.68	0.68
65	assign (segid 3A4 and resid 278 and name CA)	(segid 3A4 and resid 411 and name CB)	14.41	0.58	0.59
	assign (segid 3A4 and resid 278 and name CA)	(segid 3A4 and resid 412 and name CA)	11.73	0.89	0.89
	assign (segid 3A4 and resid 278 and name CA)	(segid 3A4 and resid 413 and name CA)	10.31	1.02	1.02
	assign (segid 3A4 and resid 278 and name CA)	(segid 3A4 and resid 414 and name CA)	11.57	0.98	0.99
	assign (segid 3A4 and resid 278 and name CA)	(segid 3A4 and resid 415 and name CA)	13.38	1.29	1.29
70	assign (segid 3A4 and resid 278 and name CA)	(segid 3A4 and resid 415 and name CB)	13.78	1.30	1.31
	assign (segid 3A4 and resid 278 and name CA)	(segid 3A4 and resid 416 and name CA)	16.03	1.51	1.50
	assign (segid 3A4 and resid 278 and name CA)	(segid 3A4 and resid 440 and name CA)	17.20	0.35	0.36
	assign (segid 3A4 and resid 278 and name CA)	(segid 3A4 and resid 279 and name C)	5.37	0.06	0.06
	assign (segid 3A4 and resid 278 and name CB)	(segid 3A4 and resid 279 and name CA)	4.42	0.04	0.03
75	assign (segid 3A4 and resid 278 and name CB)	(segid 3A4 and resid 279 and name CB)	5.22	0.05	0.05
	assign (segid 3A4 and resid 278 and name CB)	(segid 3A4 and resid 279 and name N)	3.09	0.03	0.03
	assign (segid 3A4 and resid 278 and name CB)	(segid 3A4 and resid 279 and name O)	6.24	0.10	0.10
	assign (segid 3A4 and resid 278 and name CB)	(segid 3A4 and resid 280 and name C)	6.85	0.07	0.07
	assign (segid 3A4 and resid 278 and name CB)	(segid 3A4 and resid 280 and name CA)	6.77	0.06	0.05
80	assign (segid 3A4 and resid 278 and name CB)	(segid 3A4 and resid 280 and name CB)	7.29	0.05	0.05
	assign (segid 3A4 and resid 278 and name CB)	(segid 3A4 and resid 280 and name N)	5.56	0.05	0.06
	assign (segid 3A4 and resid 278 and name CB)	(segid 3A4 and resid 281 and name C)	6.79	0.11	0.11

	assign (segid 3A4 and resid 278 and name CB)	(segid 3A4 and resid 281 and name CA)	6.41	0.12	0.11
	assign (segid 3A4 and resid 278 and name CB)	(segid 3A4 and resid 281 and name CB)	5.68	0.13	0.14
	assign (segid 3A4 and resid 278 and name CB)	(segid 3A4 and resid 281 and name N)	5.93	0.09	0.10
	assign (segid 3A4 and resid 278 and name CB)	(segid 3A4 and resid 282 and name CA)	6.88	0.10	0.11
	assign (segid 3A4 and resid 278 and name CB)	(segid 3A4 and resid 282 and name N)	6.12	0.11	0.11
5	assign (segid 3A4 and resid 278 and name CB)	(segid 3A4 and resid 303 and name CA)	14.37	0.56	0.56
	assign (segid 3A4 and resid 278 and name CB)	(segid 3A4 and resid 303 and name CB)	14.88	0.50	0.50
	assign (segid 3A4 and resid 278 and name CB)	(segid 3A4 and resid 304 and name CA)	12.02	0.14	0.13
	assign (segid 3A4 and resid 278 and name CB)	(segid 3A4 and resid 304 and name CB)	10.71	0.16	0.16
	assign (segid 3A4 and resid 278 and name CB)	(segid 3A4 and resid 305 and name CA)	12.63	0.48	0.48
10	assign (segid 3A4 and resid 278 and name CB)	(segid 3A4 and resid 305 and name CB)	13.00	0.59	0.59
	assign (segid 3A4 and resid 278 and name CB)	(segid 3A4 and resid 306 and name CA)	16.12	0.38	0.38
	assign (segid 3A4 and resid 278 and name CB)	(segid 3A4 and resid 307 and name CA)	15.20	0.27	0.26
	assign (segid 3A4 and resid 278 and name CB)	(segid 3A4 and resid 307 and name CB)	14.58	0.35	0.35
	assign (segid 3A4 and resid 278 and name CB)	(segid 3A4 and resid 308 and name CA)	13.00	0.18	0.18
15	assign (segid 3A4 and resid 278 and name CB)	(segid 3A4 and resid 308 and name CB)	11.81	0.26	0.26
	assign (segid 3A4 and resid 278 and name CB)	(segid 3A4 and resid 309 and name CA)	16.09	0.42	0.41
	assign (segid 3A4 and resid 278 and name CB)	(segid 3A4 and resid 309 and name CB)	16.83	0.47	0.46
	assign (segid 3A4 and resid 278 and name CB)	(segid 3A4 and resid 310 and name CA)	18.34	0.26	0.27
20	assign (segid 3A4 and resid 278 and name CB)	(segid 3A4 and resid 310 and name CB)	18.64	0.29	0.29
	assign (segid 3A4 and resid 278 and name CB)	(segid 3A4 and resid 311 and name CA)	16.67	0.22	0.22
	assign (segid 3A4 and resid 278 and name CB)	(segid 3A4 and resid 311 and name CB)	15.38	0.21	0.22
	assign (segid 3A4 and resid 278 and name CB)	(segid 3A4 and resid 312 and name CA)	16.75	0.33	0.34
	assign (segid 3A4 and resid 278 and name CB)	(segid 3A4 and resid 312 and name CB)	16.23	0.40	0.39
25	assign (segid 3A4 and resid 278 and name CB)	(segid 3A4 and resid 315 and name CB)	18.31	0.58	0.57
	assign (segid 3A4 and resid 278 and name CB)	(segid 3A4 and resid 362 and name CA)	17.12	0.57	0.58
	assign (segid 3A4 and resid 278 and name CB)	(segid 3A4 and resid 362 and name CB)	16.99	0.60	0.60
	assign (segid 3A4 and resid 278 and name CB)	(segid 3A4 and resid 363 and name CA)	14.50	0.41	0.41
	assign (segid 3A4 and resid 278 and name CB)	(segid 3A4 and resid 363 and name CB)	13.85	0.37	0.37
	assign (segid 3A4 and resid 278 and name CB)	(segid 3A4 and resid 364 and name CA)	13.26	0.49	0.49
30	assign (segid 3A4 and resid 278 and name CB)	(segid 3A4 and resid 364 and name CB)	14.13	0.57	0.57
	assign (segid 3A4 and resid 278 and name CB)	(segid 3A4 and resid 365 and name CA)	12.41	0.57	0.57
	assign (segid 3A4 and resid 278 and name CB)	(segid 3A4 and resid 365 and name CB)	11.18	0.57	0.57
	assign (segid 3A4 and resid 278 and name CB)	(segid 3A4 and resid 401 and name CA)	19.16	0.28	0.28
	assign (segid 3A4 and resid 278 and name CB)	(segid 3A4 and resid 402 and name CA)	17.43	0.28	0.29
35	assign (segid 3A4 and resid 278 and name CB)	(segid 3A4 and resid 402 and name CB)	18.08	0.31	0.31
	assign (segid 3A4 and resid 278 and name CB)	(segid 3A4 and resid 403 and name CA)	18.72	0.30	0.30
	assign (segid 3A4 and resid 278 and name CB)	(segid 3A4 and resid 404 and name CA)	17.81	0.40	0.39
	assign (segid 3A4 and resid 278 and name CB)	(segid 3A4 and resid 404 and name CB)	18.40	0.46	0.47
40	assign (segid 3A4 and resid 278 and name CB)	(segid 3A4 and resid 405 and name CA)	14.23	0.38	0.38
	assign (segid 3A4 and resid 278 and name CB)	(segid 3A4 and resid 405 and name CB)	13.85	0.34	0.34
	assign (segid 3A4 and resid 278 and name CB)	(segid 3A4 and resid 406 and name CA)	13.80	0.43	0.43
	assign (segid 3A4 and resid 278 and name CB)	(segid 3A4 and resid 407 and name CA)	15.63	0.36	0.37
	assign (segid 3A4 and resid 278 and name CB)	(segid 3A4 and resid 407 and name CB)	17.12	0.32	0.32
	assign (segid 3A4 and resid 278 and name CB)	(segid 3A4 and resid 408 and name CA)	14.28	0.33	0.34
45	assign (segid 3A4 and resid 278 and name CB)	(segid 3A4 and resid 408 and name CB)	14.31	0.30	0.30
	assign (segid 3A4 and resid 278 and name CB)	(segid 3A4 and resid 409 and name CA)	10.67	0.40	0.39
	assign (segid 3A4 and resid 278 and name CB)	(segid 3A4 and resid 409 and name CB)	9.70	0.27	0.26
	assign (segid 3A4 and resid 278 and name CB)	(segid 3A4 and resid 410 and name CA)	12.06	0.47	0.48
	assign (segid 3A4 and resid 278 and name CB)	(segid 3A4 and resid 411 and name CA)	14.37	0.74	0.73
50	assign (segid 3A4 and resid 278 and name CB)	(segid 3A4 and resid 411 and name CB)	15.58	0.64	0.64
	assign (segid 3A4 and resid 278 and name CB)	(segid 3A4 and resid 412 and name CA)	12.68	0.95	0.94
	assign (segid 3A4 and resid 278 and name CB)	(segid 3A4 and resid 413 and name CA)	10.80	1.04	1.04
	assign (segid 3A4 and resid 278 and name CB)	(segid 3A4 and resid 414 and name CA)	12.12	0.98	0.98
	assign (segid 3A4 and resid 278 and name CB)	(segid 3A4 and resid 415 and name CA)	13.67	1.33	1.33
55	assign (segid 3A4 and resid 278 and name CB)	(segid 3A4 and resid 415 and name CB)	13.97	1.35	1.35
	assign (segid 3A4 and resid 278 and name CB)	(segid 3A4 and resid 440 and name CA)	17.78	0.44	0.44
	assign (segid 3A4 and resid 278 and name N)	(segid 3A4 and resid 278 and name C)	2.44	0.02	0.03
	assign (segid 3A4 and resid 278 and name N)	(segid 3A4 and resid 278 and name CA)	1.46	0.01	0.00
60	assign (segid 3A4 and resid 278 and name N)	(segid 3A4 and resid 278 and name CB)	2.45	0.05	0.04
	assign (segid 3A4 and resid 278 and name N)	(segid 3A4 and resid 278 and name O)	3.48	0.04	0.04
	assign (segid 3A4 and resid 278 and name N)	(segid 3A4 and resid 279 and name C)	4.66	0.04	0.04
	assign (segid 3A4 and resid 278 and name N)	(segid 3A4 and resid 279 and name CB)	4.18	0.03	0.02
	assign (segid 3A4 and resid 278 and name N)	(segid 3A4 and resid 279 and name N)	4.85	0.08	0.09
65	assign (segid 3A4 and resid 278 and name N)	(segid 3A4 and resid 279 and name O)	2.79	0.03	0.03
	assign (segid 3A4 and resid 278 and name N)	(segid 3A4 and resid 279 and name O)	5.74	0.07	0.07
	assign (segid 3A4 and resid 278 and name N)	(segid 3A4 and resid 280 and name C)	5.57	0.06	0.06
	assign (segid 3A4 and resid 278 and name N)	(segid 3A4 and resid 280 and name CA)	5.27	0.03	0.04
	assign (segid 3A4 and resid 278 and name N)	(segid 3A4 and resid 280 and name CB)	5.38	0.10	0.09
70	assign (segid 3A4 and resid 278 and name N)	(segid 3A4 and resid 280 and name N)	4.26	0.04	0.04
	assign (segid 3A4 and resid 278 and name N)	(segid 3A4 and resid 280 and name O)	6.78	0.07	0.06
	assign (segid 3A4 and resid 278 and name N)	(segid 3A4 and resid 281 and name C)	6.39	0.08	0.09
	assign (segid 3A4 and resid 278 and name N)	(segid 3A4 and resid 281 and name CA)	5.55	0.07	0.06
	assign (segid 3A4 and resid 278 and name N)	(segid 3A4 and resid 281 and name CB)	4.98	0.06	0.07
	assign (segid 3A4 and resid 278 and name N)	(segid 3A4 and resid 281 and name N)	4.75	0.06	0.06
75	assign (segid 3A4 and resid 278 and name N)	(segid 3A4 and resid 281 and name O)	7.58	0.10	0.10
	assign (segid 3A4 and resid 278 and name N)	(segid 3A4 and resid 282 and name CA)	7.18	0.11	0.11
	assign (segid 3A4 and resid 278 and name N)	(segid 3A4 and resid 282 and name N)	6.05	0.09	0.08
	assign (segid 3A4 and resid 278 and name N)	(segid 3A4 and resid 409 and name CD2)	7.22	0.59	0.59
80	assign (segid 3A4 and resid 278 and name O)	(segid 3A4 and resid 278 and name CB)	3.29	0.05	0.05
	assign (segid 3A4 and resid 278 and name O)	(segid 3A4 and resid 279 and name C)	2.95	0.06	0.05
	assign (segid 3A4 and resid 278 and name O)	(segid 3A4 and resid 279 and name CA)	2.76	0.03	0.04
	assign (segid 3A4 and resid 278 and name O)	(segid 3A4 and resid 279 and name CB)	4.23	0.05	0.05

	assign (segid 3A4 and resid 278 and name O) (segid 3A4 and resid 279 and name N)	2.25	0.01	0.01
	assign (segid 3A4 and resid 278 and name O) (segid 3A4 and resid 279 and name O)	3.41	0.10	0.11
	assign (segid 3A4 and resid 278 and name O) (segid 3A4 and resid 280 and name C)	4.08	0.07	0.07
	assign (segid 3A4 and resid 278 and name O) (segid 3A4 and resid 280 and name CA)	4.36	0.08	0.08
	assign (segid 3A4 and resid 278 and name O) (segid 3A4 and resid 280 and name CB)	5.37	0.06	0.06
5	assign (segid 3A4 and resid 278 and name O) (segid 3A4 and resid 280 and name N)	3.42	0.08	0.07
	assign (segid 3A4 and resid 278 and name O) (segid 3A4 and resid 280 and name O)	5.00	0.06	0.07
	assign (segid 3A4 and resid 278 and name O) (segid 3A4 and resid 281 and name C)	3.79	0.07	0.07
	assign (segid 3A4 and resid 278 and name O) (segid 3A4 and resid 281 and name CA)	3.75	0.12	0.11
	assign (segid 3A4 and resid 278 and name O) (segid 3A4 and resid 281 and name CB)	3.65	0.15	0.15
10	assign (segid 3A4 and resid 278 and name O) (segid 3A4 and resid 281 and name N)	3.29	0.11	0.10
	assign (segid 3A4 and resid 278 and name O) (segid 3A4 and resid 281 and name O)	4.96	0.06	0.06
	assign (segid 3A4 and resid 278 and name O) (segid 3A4 and resid 282 and name C)	4.93	0.06	0.06
	assign (segid 3A4 and resid 278 and name O) (segid 3A4 and resid 282 and name CA)	3.81	0.08	0.08
	assign (segid 3A4 and resid 278 and name O) (segid 3A4 and resid 282 and name N)	2.95	0.05	0.06
15	assign (segid 3A4 and resid 278 and name O) (segid 3A4 and resid 282 and name O)	6.04	0.04	0.04
	assign (segid 3A4 and resid 279 and name C) (segid 3A4 and resid 279 and name CB)	2.53	0.04	0.03
	assign (segid 3A4 and resid 279 and name C) (segid 3A4 and resid 279 and name O)	1.24	0.01	0.00
	assign (segid 3A4 and resid 279 and name C) (segid 3A4 and resid 280 and name C)	3.05	0.04	0.05
	assign (segid 3A4 and resid 279 and name C) (segid 3A4 and resid 280 and name CA)	2.44	0.01	0.01
20	assign (segid 3A4 and resid 279 and name C) (segid 3A4 and resid 280 and name CB)	3.71	0.03	0.03
	assign (segid 3A4 and resid 279 and name C) (segid 3A4 and resid 280 and name N)	1.33	0.00	0.01
	assign (segid 3A4 and resid 279 and name C) (segid 3A4 and resid 280 and name O)	3.91	0.10	0.10
	assign (segid 3A4 and resid 279 and name C) (segid 3A4 and resid 281 and name C)	4.61	0.08	0.08
	assign (segid 3A4 and resid 279 and name C) (segid 3A4 and resid 281 and name CA)	4.52	0.08	0.07
25	assign (segid 3A4 and resid 279 and name C) (segid 3A4 and resid 281 and name CB)	5.26	0.08	0.08
	assign (segid 3A4 and resid 279 and name C) (segid 3A4 and resid 281 and name N)	3.32	0.07	0.08
	assign (segid 3A4 and resid 279 and name C) (segid 3A4 and resid 281 and name O)	5.71	0.09	0.09
	assign (segid 3A4 and resid 279 and name C) (segid 3A4 and resid 282 and name C)	4.87	0.09	0.09
	assign (segid 3A4 and resid 279 and name C) (segid 3A4 and resid 282 and name CA)	4.59	0.12	0.12
30	assign (segid 3A4 and resid 279 and name C) (segid 3A4 and resid 282 and name N)	3.85	0.09	0.10
	assign (segid 3A4 and resid 279 and name C) (segid 3A4 and resid 282 and name O)	6.05	0.10	0.11
	assign (segid 3A4 and resid 279 and name C) (segid 3A4 and resid 304 and name C)	7.01	0.23	0.23
	assign (segid 3A4 and resid 279 and name C) (segid 3A4 and resid 304 and name CA)	6.79	0.17	0.17
35	assign (segid 3A4 and resid 279 and name C) (segid 3A4 and resid 304 and name CB)	5.50	0.22	0.22
	assign (segid 3A4 and resid 279 and name C) (segid 3A4 and resid 304 and name N)	7.25	0.32	0.32
	assign (segid 3A4 and resid 279 and name C) (segid 3A4 and resid 304 and name O)	7.32	0.30	0.30
	assign (segid 3A4 and resid 279 and name C) (segid 3A4 and resid 305 and name N)	7.24	0.34	0.33
	assign (segid 3A4 and resid 279 and name C) (segid 3A4 and resid 279 and name C)	1.53	0.01	0.02
	assign (segid 3A4 and resid 279 and name CA) (segid 3A4 and resid 279 and name CB)	1.52	0.01	0.01
40	assign (segid 3A4 and resid 279 and name CA) (segid 3A4 and resid 279 and name O)	2.41	0.02	0.03
	assign (segid 3A4 and resid 279 and name CA) (segid 3A4 and resid 280 and name C)	4.45	0.05	0.05
	assign (segid 3A4 and resid 279 and name CA) (segid 3A4 and resid 280 and name CA)	3.83	0.03	0.03
	assign (segid 3A4 and resid 279 and name CA) (segid 3A4 and resid 280 and name CB)	4.88	0.04	0.04
	assign (segid 3A4 and resid 279 and name CA) (segid 3A4 and resid 280 and name N)	2.45	0.02	0.02
45	assign (segid 3A4 and resid 279 and name CA) (segid 3A4 and resid 280 and name O)	5.38	0.10	0.10
	assign (segid 3A4 and resid 279 and name CA) (segid 3A4 and resid 281 and name C)	5.55	0.11	0.12
	assign (segid 3A4 and resid 279 and name CA) (segid 3A4 and resid 281 and name CA)	5.50	0.10	0.09
	assign (segid 3A4 and resid 279 and name CA) (segid 3A4 and resid 281 and name CB)	5.91	0.10	0.10
	assign (segid 3A4 and resid 279 and name CA) (segid 3A4 and resid 281 and name N)	4.42	0.08	0.07
50	assign (segid 3A4 and resid 279 and name CA) (segid 3A4 and resid 281 and name O)	6.70	0.12	0.13
	assign (segid 3A4 and resid 279 and name CA) (segid 3A4 and resid 282 and name C)	5.72	0.11	0.11
	assign (segid 3A4 and resid 279 and name CA) (segid 3A4 and resid 282 and name CA)	5.19	0.18	0.17
	assign (segid 3A4 and resid 279 and name CA) (segid 3A4 and resid 282 and name N)	4.61	0.14	0.14
	assign (segid 3A4 and resid 279 and name CA) (segid 3A4 and resid 282 and name O)	6.86	0.12	0.12
55	assign (segid 3A4 and resid 279 and name CA) (segid 3A4 and resid 303 and name C)	10.36	0.43	0.42
	assign (segid 3A4 and resid 279 and name CA) (segid 3A4 and resid 303 and name CB)	10.79	0.38	0.38
	assign (segid 3A4 and resid 279 and name CA) (segid 3A4 and resid 304 and name CA)	7.85	0.17	0.16
	assign (segid 3A4 and resid 279 and name CA) (segid 3A4 and resid 304 and name CB)	6.46	0.18	0.18
	assign (segid 3A4 and resid 279 and name CA) (segid 3A4 and resid 305 and name CA)	9.17	0.51	0.51
60	assign (segid 3A4 and resid 279 and name CA) (segid 3A4 and resid 305 and name CB)	9.76	0.64	0.63
	assign (segid 3A4 and resid 279 and name CA) (segid 3A4 and resid 306 and name CA)	12.44	0.34	0.34
	assign (segid 3A4 and resid 279 and name CA) (segid 3A4 and resid 307 and name CA)	11.42	0.13	0.13
	assign (segid 3A4 and resid 279 and name CA) (segid 3A4 and resid 307 and name CB)	10.65	0.25	0.24
	assign (segid 3A4 and resid 279 and name CA) (segid 3A4 and resid 308 and name CA)	9.94	0.21	0.21
65	assign (segid 3A4 and resid 279 and name CA) (segid 3A4 and resid 308 and name CB)	8.89	0.29	0.30
	assign (segid 3A4 and resid 279 and name CA) (segid 3A4 and resid 309 and name CA)	13.29	0.38	0.38
	assign (segid 3A4 and resid 279 and name CA) (segid 3A4 and resid 309 and name CB)	13.93	0.40	0.41
	assign (segid 3A4 and resid 279 and name CA) (segid 3A4 and resid 310 and name CA)	15.20	0.22	0.22
	assign (segid 3A4 and resid 279 and name CA) (segid 3A4 and resid 310 and name CB)	15.26	0.20	0.19
70	assign (segid 3A4 and resid 279 and name CA) (segid 3A4 and resid 311 and name CA)	13.98	0.38	0.38
	assign (segid 3A4 and resid 279 and name CA) (segid 3A4 and resid 311 and name CB)	12.69	0.40	0.40
	assign (segid 3A4 and resid 279 and name CA) (segid 3A4 and resid 312 and name CA)	14.77	0.48	0.49
	assign (segid 3A4 and resid 279 and name CA) (segid 3A4 and resid 312 and name CB)	14.34	0.52	0.52
	assign (segid 3A4 and resid 279 and name CA) (segid 3A4 and resid 313 and name CA)	18.15	0.41	0.40
75	assign (segid 3A4 and resid 279 and name CA) (segid 3A4 and resid 313 and name CB)	18.52	0.37	0.38
	assign (segid 3A4 and resid 279 and name CA) (segid 3A4 and resid 314 and name CA)	18.76	0.42	0.43
	assign (segid 3A4 and resid 279 and name CA) (segid 3A4 and resid 314 and name CB)	18.11	0.39	0.40
	assign (segid 3A4 and resid 279 and name CA) (segid 3A4 and resid 315 and name CA)	18.09	0.69	0.69
	assign (segid 3A4 and resid 279 and name CA) (segid 3A4 and resid 315 and name CB)	16.79	0.76	0.75
80	assign (segid 3A4 and resid 279 and name CA) (segid 3A4 and resid 362 and name CA)	16.15	0.77	0.77
	assign (segid 3A4 and resid 279 and name CA) (segid 3A4 and resid 362 and name CB)	15.97	0.77	0.77
	assign (segid 3A4 and resid 279 and name CA) (segid 3A4 and resid 363 and name CA)	13.24	0.68	0.67

	assign (segid 3A4 and resid 279 and name CA) (segid 3A4 and resid 363 and name CB)	12.88	0.67	0.66
	assign (segid 3A4 and resid 279 and name CA) (segid 3A4 and resid 364 and name CA)	11.15	0.69	0.70
	assign (segid 3A4 and resid 279 and name CA) (segid 3A4 and resid 364 and name CB)	12.02	0.74	0.75
	assign (segid 3A4 and resid 279 and name CA) (segid 3A4 and resid 365 and name CA)	9.35	0.76	0.76
5	assign (segid 3A4 and resid 279 and name CA) (segid 3A4 and resid 365 and name CB)	8.06	0.73	0.72
	assign (segid 3A4 and resid 279 and name CA) (segid 3A4 and resid 401 and name CA)	17.03	0.26	0.26
	assign (segid 3A4 and resid 279 and name CA) (segid 3A4 and resid 402 and name CA)	14.83	0.21	0.20
	assign (segid 3A4 and resid 279 and name CA) (segid 3A4 and resid 402 and name CB)	15.19	0.23	0.22
	assign (segid 3A4 and resid 279 and name CA) (segid 3A4 and resid 403 and name CA)	16.60	0.23	0.23
	assign (segid 3A4 and resid 279 and name CA) (segid 3A4 and resid 403 and name CB)	18.12	0.23	0.23
10	assign (segid 3A4 and resid 279 and name CA) (segid 3A4 and resid 404 and name CA)	16.45	0.45	0.44
	assign (segid 3A4 and resid 279 and name CA) (segid 3A4 and resid 404 and name CB)	17.11	0.51	0.52
	assign (segid 3A4 and resid 279 and name CA) (segid 3A4 and resid 405 and name CA)	12.84	0.53	0.52
	assign (segid 3A4 and resid 279 and name CA) (segid 3A4 and resid 405 and name CB)	12.19	0.49	0.50
	assign (segid 3A4 and resid 279 and name CA) (segid 3A4 and resid 406 and name CA)	12.05	0.46	0.45
15	assign (segid 3A4 and resid 279 and name CA) (segid 3A4 and resid 407 and name CA)	14.72	0.54	0.55
	assign (segid 3A4 and resid 279 and name CA) (segid 3A4 and resid 407 and name CB)	16.17	0.51	0.51
	assign (segid 3A4 and resid 279 and name CA) (segid 3A4 and resid 408 and name CA)	14.24	0.41	0.40
	assign (segid 3A4 and resid 279 and name CA) (segid 3A4 and resid 408 and name CB)	14.27	0.41	0.41
	assign (segid 3A4 and resid 279 and name CA) (segid 3A4 and resid 409 and name CA)	10.85	0.45	0.46
20	assign (segid 3A4 and resid 279 and name CA) (segid 3A4 and resid 409 and name CB)	9.56	0.42	0.42
	assign (segid 3A4 and resid 279 and name CA) (segid 3A4 and resid 410 and name CA)	12.10	0.39	0.38
	assign (segid 3A4 and resid 279 and name CA) (segid 3A4 and resid 411 and name CA)	15.17	0.54	0.53
	assign (segid 3A4 and resid 279 and name CA) (segid 3A4 and resid 411 and name CB)	16.24	0.45	0.45
	assign (segid 3A4 and resid 279 and name CA) (segid 3A4 and resid 412 and name CA)	14.34	0.74	0.75
25	assign (segid 3A4 and resid 279 and name CA) (segid 3A4 and resid 413 and name CA)	13.61	1.00	0.99
	assign (segid 3A4 and resid 279 and name CA) (segid 3A4 and resid 414 and name CA)	14.63	0.88	0.88
	assign (segid 3A4 and resid 279 and name CA) (segid 3A4 and resid 415 and name CA)	16.46	1.05	1.06
	assign (segid 3A4 and resid 279 and name CA) (segid 3A4 and resid 415 and name CB)	16.96	1.00	1.00
	assign (segid 3A4 and resid 279 and name CA) (segid 3A4 and resid 280 and name C)	5.47	0.05	0.05
30	assign (segid 3A4 and resid 279 and name CB) (segid 3A4 and resid 280 and name CA)	4.50	0.08	0.07
	assign (segid 3A4 and resid 279 and name CB) (segid 3A4 and resid 280 and name CB)	5.32	0.13	0.14
	assign (segid 3A4 and resid 279 and name CB) (segid 3A4 and resid 280 and name N)	3.16	0.06	0.06
	assign (segid 3A4 and resid 279 and name CB) (segid 3A4 and resid 280 and name O)	6.37	0.09	0.09
	assign (segid 3A4 and resid 279 and name CB) (segid 3A4 and resid 281 and name C)	6.97	0.11	0.11
35	assign (segid 3A4 and resid 279 and name CB) (segid 3A4 and resid 281 and name CA)	6.84	0.07	0.08
	assign (segid 3A4 and resid 279 and name CB) (segid 3A4 and resid 281 and name CB)	7.30	0.07	0.08
	assign (segid 3A4 and resid 279 and name CB) (segid 3A4 and resid 281 and name N)	5.64	0.06	0.05
	assign (segid 3A4 and resid 279 and name CB) (segid 3A4 and resid 282 and name C)	6.93	0.16	0.17
	assign (segid 3A4 and resid 279 and name CB) (segid 3A4 and resid 282 and name CA)	6.57	0.22	0.23
40	assign (segid 3A4 and resid 279 and name CB) (segid 3A4 and resid 282 and name N)	6.06	0.16	0.16
	assign (segid 3A4 and resid 279 and name CB) (segid 3A4 and resid 303 and name CA)	10.43	0.27	0.27
	assign (segid 3A4 and resid 279 and name CB) (segid 3A4 and resid 303 and name CB)	10.82	0.23	0.23
	assign (segid 3A4 and resid 279 and name CB) (segid 3A4 and resid 304 and name CA)	7.55	0.27	0.28
	assign (segid 3A4 and resid 279 and name CB) (segid 3A4 and resid 304 and name CB)	6.12	0.26	0.26
45	assign (segid 3A4 and resid 279 and name CB) (segid 3A4 and resid 305 and name CA)	9.12	0.52	0.52
	assign (segid 3A4 and resid 279 and name CB) (segid 3A4 and resid 305 and name CB)	9.91	0.63	0.63
	assign (segid 3A4 and resid 279 and name CB) (segid 3A4 and resid 306 and name CA)	12.10	0.34	0.34
	assign (segid 3A4 and resid 279 and name CB) (segid 3A4 and resid 307 and name CA)	10.66	0.15	0.14
	assign (segid 3A4 and resid 279 and name CB) (segid 3A4 and resid 307 and name CB)	9.82	0.25	0.24
50	assign (segid 3A4 and resid 279 and name CB) (segid 3A4 and resid 308 and name CA)	9.26	0.31	0.30
	assign (segid 3A4 and resid 279 and name CB) (segid 3A4 and resid 308 and name CB)	8.37	0.39	0.39
	assign (segid 3A4 and resid 279 and name CB) (segid 3A4 and resid 309 and name CA)	12.78	0.42	0.42
	assign (segid 3A4 and resid 279 and name CB) (segid 3A4 and resid 309 and name CB)	13.55	0.43	0.42
	assign (segid 3A4 and resid 279 and name CB) (segid 3A4 and resid 310 and name CA)	14.40	0.28	0.27
55	assign (segid 3A4 and resid 279 and name CB) (segid 3A4 and resid 310 and name CB)	14.41	0.23	0.22
	assign (segid 3A4 and resid 279 and name CB) (segid 3A4 and resid 311 and name CA)	12.96	0.48	0.49
	assign (segid 3A4 and resid 279 and name CB) (segid 3A4 and resid 311 and name CB)	11.62	0.50	0.50
	assign (segid 3A4 and resid 279 and name CB) (segid 3A4 and resid 312 and name CA)	13.99	0.62	0.63
	assign (segid 3A4 and resid 279 and name CB) (segid 3A4 and resid 312 and name CB)	13.70	0.67	0.66
60	assign (segid 3A4 and resid 279 and name CB) (segid 3A4 and resid 313 and name CA)	17.37	0.53	0.53
	assign (segid 3A4 and resid 279 and name CB) (segid 3A4 and resid 313 and name CB)	17.78	0.49	0.48
	assign (segid 3A4 and resid 279 and name CB) (segid 3A4 and resid 314 and name CA)	17.73	0.55	0.55
	assign (segid 3A4 and resid 279 and name CB) (segid 3A4 and resid 314 and name CB)	17.01	0.51	0.51
	assign (segid 3A4 and resid 279 and name CB) (segid 3A4 and resid 315 and name CA)	17.05	0.83	0.82
65	assign (segid 3A4 and resid 279 and name CB) (segid 3A4 and resid 315 and name CB)	15.75	0.89	0.88
	assign (segid 3A4 and resid 279 and name CB) (segid 3A4 and resid 359 and name CA)	18.46	0.60	0.60
	assign (segid 3A4 and resid 279 and name CB) (segid 3A4 and resid 359 and name CB)	17.47	0.72	0.71
	assign (segid 3A4 and resid 279 and name CB) (segid 3A4 and resid 362 and name CA)	14.85	0.87	0.88
	assign (segid 3A4 and resid 279 and name CB) (segid 3A4 and resid 362 and name CB)	14.62	0.85	0.85
70	assign (segid 3A4 and resid 279 and name CB) (segid 3A4 and resid 363 and name CA)	12.03	0.80	0.80
	assign (segid 3A4 and resid 279 and name CB) (segid 3A4 and resid 363 and name CB)	11.77	0.80	0.80
	assign (segid 3A4 and resid 279 and name CB) (segid 3A4 and resid 364 and name CA)	9.78	0.76	0.76
	assign (segid 3A4 and resid 279 and name CB) (segid 3A4 and resid 364 and name CB)	10.59	0.80	0.80
	assign (segid 3A4 and resid 279 and name CB) (segid 3A4 and resid 365 and name CA)	8.11	0.80	0.80
75	assign (segid 3A4 and resid 279 and name CB) (segid 3A4 and resid 365 and name CB)	6.91	0.76	0.76
	assign (segid 3A4 and resid 279 and name CB) (segid 3A4 and resid 401 and name CA)	17.06	0.39	0.39
	assign (segid 3A4 and resid 279 and name CB) (segid 3A4 and resid 402 and name CA)	14.98	0.29	0.29
	assign (segid 3A4 and resid 279 and name CB) (segid 3A4 and resid 402 and name CB)	15.29	0.26	0.26
	assign (segid 3A4 and resid 279 and name CB) (segid 3A4 and resid 403 and name CA)	17.05	0.29	0.29
80	assign (segid 3A4 and resid 279 and name CB) (segid 3A4 and resid 403 and name CB)	18.57	0.28	0.28
	assign (segid 3A4 and resid 279 and name CB) (segid 3A4 and resid 404 and name CA)	16.91	0.56	0.57
	assign (segid 3A4 and resid 279 and name CB) (segid 3A4 and resid 404 and name CB)	17.49	0.66	0.66

	assign (segid 3A4 and resid 279 and name CB)	(segid 3A4 and resid 405 and name CA)	13.26	0.64	0.65
	assign (segid 3A4 and resid 279 and name CB)	(segid 3A4 and resid 405 and name CB)	12.48	0.64	0.63
	assign (segid 3A4 and resid 279 and name CB)	(segid 3A4 and resid 406 and name CA)	12.75	0.48	0.49
	assign (segid 3A4 and resid 279 and name CB)	(segid 3A4 and resid 407 and name CA)	15.61	0.53	0.53
5	assign (segid 3A4 and resid 279 and name CB)	(segid 3A4 and resid 407 and name CB)	17.02	0.50	0.50
	assign (segid 3A4 and resid 279 and name CB)	(segid 3A4 and resid 408 and name CA)	15.08	0.39	0.38
	assign (segid 3A4 and resid 279 and name CB)	(segid 3A4 and resid 408 and name CB)	14.99	0.43	0.43
	assign (segid 3A4 and resid 279 and name CB)	(segid 3A4 and resid 409 and name CA)	11.84	0.41	0.42
	assign (segid 3A4 and resid 279 and name CB)	(segid 3A4 and resid 409 and name CB)	10.49	0.38	0.39
10	assign (segid 3A4 and resid 279 and name CB)	(segid 3A4 and resid 410 and name CA)	13.32	0.32	0.31
	assign (segid 3A4 and resid 279 and name CB)	(segid 3A4 and resid 411 and name CA)	16.36	0.47	0.47
	assign (segid 3A4 and resid 279 and name CB)	(segid 3A4 and resid 411 and name CB)	17.38	0.38	0.38
	assign (segid 3A4 and resid 279 and name CB)	(segid 3A4 and resid 412 and name CA)	15.45	0.75	0.75
	assign (segid 3A4 and resid 279 and name CB)	(segid 3A4 and resid 413 and name CA)	14.54	0.95	0.94
15	assign (segid 3A4 and resid 279 and name CB)	(segid 3A4 and resid 414 and name CA)	15.28	0.75	0.74
	assign (segid 3A4 and resid 279 and name CB)	(segid 3A4 and resid 415 and name CA)	16.89	0.86	0.85
	assign (segid 3A4 and resid 279 and name CB)	(segid 3A4 and resid 415 and name CB)	17.40	0.78	0.78
	assign (segid 3A4 and resid 279 and name CB)	(segid 3A4 and resid 279 and name C)	2.46	0.02	0.02
	assign (segid 3A4 and resid 279 and name N)	(segid 3A4 and resid 279 and name C)	1.45	0.00	0.01
	assign (segid 3A4 and resid 279 and name N)	(segid 3A4 and resid 279 and name CB)	2.40	0.05	0.04
20	assign (segid 3A4 and resid 279 and name N)	(segid 3A4 and resid 279 and name O)	3.50	0.02	0.03
	assign (segid 3A4 and resid 279 and name N)	(segid 3A4 and resid 280 and name C)	4.72	0.02	0.03
	assign (segid 3A4 and resid 279 and name N)	(segid 3A4 and resid 280 and name CA)	4.23	0.05	0.05
	assign (segid 3A4 and resid 279 and name N)	(segid 3A4 and resid 280 and name CB)	5.01	0.03	0.02
25	assign (segid 3A4 and resid 279 and name N)	(segid 3A4 and resid 280 and name N)	2.82	0.06	0.06
	assign (segid 3A4 and resid 279 and name N)	(segid 3A4 and resid 280 and name O)	5.82	0.05	0.04
	assign (segid 3A4 and resid 279 and name N)	(segid 3A4 and resid 281 and name C)	5.64	0.06	0.05
	assign (segid 3A4 and resid 279 and name N)	(segid 3A4 and resid 281 and name CA)	5.33	0.06	0.06
	assign (segid 3A4 and resid 279 and name N)	(segid 3A4 and resid 281 and name CB)	5.38	0.08	0.09
30	assign (segid 3A4 and resid 279 and name N)	(segid 3A4 and resid 281 and name N)	4.33	0.06	0.05
	assign (segid 3A4 and resid 279 and name N)	(segid 3A4 and resid 281 and name O)	6.85	0.06	0.06
	assign (segid 3A4 and resid 279 and name N)	(segid 3A4 and resid 282 and name C)	6.43	0.07	0.07
	assign (segid 3A4 and resid 279 and name N)	(segid 3A4 and resid 282 and name CA)	5.62	0.12	0.12
	assign (segid 3A4 and resid 279 and name N)	(segid 3A4 and resid 282 and name N)	4.82	0.08	0.08
35	assign (segid 3A4 and resid 279 and name N)	(segid 3A4 and resid 282 and name O)	7.59	0.07	0.08
	assign (segid 3A4 and resid 279 and name O)	(segid 3A4 and resid 279 and name CB)	3.36	0.09	0.08
	assign (segid 3A4 and resid 279 and name O)	(segid 3A4 and resid 280 and name C)	3.02	0.09	0.08
	assign (segid 3A4 and resid 279 and name O)	(segid 3A4 and resid 280 and name CA)	2.76	0.03	0.04
	assign (segid 3A4 and resid 279 and name O)	(segid 3A4 and resid 280 and name CB)	4.24	0.03	0.03
40	assign (segid 3A4 and resid 279 and name O)	(segid 3A4 and resid 280 and name N)	2.25	0.02	0.02
	assign (segid 3A4 and resid 279 and name O)	(segid 3A4 and resid 280 and name O)	3.52	0.16	0.16
	assign (segid 3A4 and resid 279 and name O)	(segid 3A4 and resid 281 and name C)	4.21	0.11	0.12
	assign (segid 3A4 and resid 279 and name O)	(segid 3A4 and resid 281 and name CA)	4.47	0.13	0.12
	assign (segid 3A4 and resid 279 and name O)	(segid 3A4 and resid 281 and name CB)	5.44	0.11	0.12
45	assign (segid 3A4 and resid 279 and name O)	(segid 3A4 and resid 281 and name N)	3.50	0.10	0.10
	assign (segid 3A4 and resid 279 and name O)	(segid 3A4 and resid 281 and name O)	5.16	0.09	0.10
	assign (segid 3A4 and resid 279 and name O)	(segid 3A4 and resid 282 and name C)	3.85	0.09	0.09
	assign (segid 3A4 and resid 279 and name O)	(segid 3A4 and resid 282 and name CA)	3.85	0.12	0.12
	assign (segid 3A4 and resid 279 and name O)	(segid 3A4 and resid 282 and name N)	3.39	0.14	0.13
50	assign (segid 3A4 and resid 279 and name O)	(segid 3A4 and resid 282 and name O)	4.99	0.11	0.11
	assign (segid 3A4 and resid 279 and name O)	(segid 3A4 and resid 304 and name C)	6.75	0.22	0.21
	assign (segid 3A4 and resid 279 and name O)	(segid 3A4 and resid 304 and name CA)	6.35	0.23	0.23
	assign (segid 3A4 and resid 279 and name O)	(segid 3A4 and resid 304 and name CB)	5.08	0.23	0.24
	assign (segid 3A4 and resid 279 and name O)	(segid 3A4 and resid 304 and name N)	6.61	0.40	0.40
55	assign (segid 3A4 and resid 279 and name O)	(segid 3A4 and resid 304 and name O)	7.24	0.29	0.29
	assign (segid 3A4 and resid 279 and name O)	(segid 3A4 and resid 305 and name N)	6.92	0.33	0.33
	assign (segid 3A4 and resid 280 and name C)	(segid 3A4 and resid 280 and name CB)	2.49	0.03	0.04
	assign (segid 3A4 and resid 280 and name C)	(segid 3A4 and resid 280 and name O)	1.24	0.01	0.00
	assign (segid 3A4 and resid 280 and name C)	(segid 3A4 and resid 281 and name C)	3.05	0.04	0.04
60	assign (segid 3A4 and resid 280 and name C)	(segid 3A4 and resid 281 and name CA)	2.44	0.01	0.01
	assign (segid 3A4 and resid 280 and name C)	(segid 3A4 and resid 281 and name CB)	3.72	0.01	0.02
	assign (segid 3A4 and resid 280 and name C)	(segid 3A4 and resid 281 and name N)	1.33	0.01	0.01
	assign (segid 3A4 and resid 280 and name C)	(segid 3A4 and resid 281 and name O)	3.93	0.08	0.08
	assign (segid 3A4 and resid 280 and name C)	(segid 3A4 and resid 282 and name C)	4.56	0.07	0.07
	assign (segid 3A4 and resid 280 and name C)	(segid 3A4 and resid 282 and name CA)	4.47	0.05	0.06
65	assign (segid 3A4 and resid 280 and name C)	(segid 3A4 and resid 282 and name N)	3.29	0.04	0.04
	assign (segid 3A4 and resid 280 and name C)	(segid 3A4 and resid 282 and name O)	5.64	0.13	0.12
	assign (segid 3A4 and resid 280 and name C)	(segid 3A4 and resid 304 and name C)	6.71	0.27	0.27
	assign (segid 3A4 and resid 280 and name C)	(segid 3A4 and resid 304 and name CA)	6.89	0.39	0.38
	assign (segid 3A4 and resid 280 and name C)	(segid 3A4 and resid 304 and name CB)	6.08	0.41	0.41
70	assign (segid 3A4 and resid 280 and name C)	(segid 3A4 and resid 304 and name N)	7.23	0.31	0.32
	assign (segid 3A4 and resid 280 and name C)	(segid 3A4 and resid 305 and name CA)	6.67	0.36	0.37
	assign (segid 3A4 and resid 280 and name C)	(segid 3A4 and resid 305 and name CB)	6.62	0.52	0.53
	assign (segid 3A4 and resid 280 and name C)	(segid 3A4 and resid 305 and name N)	6.38	0.22	0.21
	assign (segid 3A4 and resid 280 and name C)	(segid 3A4 and resid 409 and name CB)	5.98	0.62	0.61
75	assign (segid 3A4 and resid 280 and name C)	(segid 3A4 and resid 409 and name CG)	6.30	0.74	0.73
	assign (segid 3A4 and resid 280 and name CA)	(segid 3A4 and resid 280 and name C)	1.52	0.00	0.01
	assign (segid 3A4 and resid 280 and name CA)	(segid 3A4 and resid 280 and name CB)	1.53	0.02	0.01
	assign (segid 3A4 and resid 280 and name CA)	(segid 3A4 and resid 280 and name O)	2.39	0.01	0.01
80	assign (segid 3A4 and resid 280 and name CA)	(segid 3A4 and resid 281 and name C)	4.43	0.03	0.04
	assign (segid 3A4 and resid 280 and name CA)	(segid 3A4 and resid 281 and name CA)	3.81	0.01	0.02
	assign (segid 3A4 and resid 280 and name CA)	(segid 3A4 and resid 281 and name CB)	4.86	0.02	0.03
	assign (segid 3A4 and resid 280 and name CA)	(segid 3A4 and resid 281 and name N)	2.43	0.02	0.02

	assign (segid 3A4 and resid 280 and name CA)	(segid 3A4 and resid 281 and name O)	5.38	0.07	0.08
	assign (segid 3A4 and resid 280 and name CA)	(segid 3A4 and resid 282 and name C)	5.49	0.05	0.04
	assign (segid 3A4 and resid 280 and name CA)	(segid 3A4 and resid 282 and name CA)	5.46	0.06	0.05
	assign (segid 3A4 and resid 280 and name CA)	(segid 3A4 and resid 282 and name N)	4.38	0.04	0.03
	assign (segid 3A4 and resid 280 and name CA)	(segid 3A4 and resid 282 and name O)	6.61	0.06	0.06
5	assign (segid 3A4 and resid 280 and name CA)	(segid 3A4 and resid 303 and name CA)	8.31	0.61	0.61
	assign (segid 3A4 and resid 280 and name CA)	(segid 3A4 and resid 303 and name CB)	9.20	0.57	0.57
	assign (segid 3A4 and resid 280 and name CA)	(segid 3A4 and resid 304 and name C)	5.84	0.23	0.23
	assign (segid 3A4 and resid 280 and name CA)	(segid 3A4 and resid 304 and name CA)	6.08	0.31	0.30
	assign (segid 3A4 and resid 280 and name CA)	(segid 3A4 and resid 304 and name CB)	5.17	0.39	0.38
10	assign (segid 3A4 and resid 280 and name CA)	(segid 3A4 and resid 304 and name N)	6.50	0.48	0.47
	assign (segid 3A4 and resid 280 and name CA)	(segid 3A4 and resid 304 and name O)	6.17	0.31	0.31
	assign (segid 3A4 and resid 280 and name CA)	(segid 3A4 and resid 305 and name CA)	6.03	0.42	0.42
	assign (segid 3A4 and resid 280 and name CA)	(segid 3A4 and resid 305 and name CB)	6.30	0.58	0.58
	assign (segid 3A4 and resid 280 and name CA)	(segid 3A4 and resid 305 and name N)	5.73	0.24	0.23
15	assign (segid 3A4 and resid 280 and name CA)	(segid 3A4 and resid 306 and name CA)	9.68	0.34	0.35
	assign (segid 3A4 and resid 280 and name CA)	(segid 3A4 and resid 307 and name CA)	9.64	0.28	0.28
	assign (segid 3A4 and resid 280 and name CA)	(segid 3A4 and resid 307 and name CB)	9.28	0.39	0.39
	assign (segid 3A4 and resid 280 and name CA)	(segid 3A4 and resid 308 and name CA)	7.90	0.16	0.16
	assign (segid 3A4 and resid 280 and name CA)	(segid 3A4 and resid 308 and name CB)	6.57	0.15	0.16
20	assign (segid 3A4 and resid 280 and name CA)	(segid 3A4 and resid 309 and name CA)	10.61	0.31	0.31
	assign (segid 3A4 and resid 280 and name CA)	(segid 3A4 and resid 309 and name CB)	10.99	0.38	0.38
	assign (segid 3A4 and resid 280 and name CA)	(segid 3A4 and resid 310 and name CA)	13.14	0.22	0.22
	assign (segid 3A4 and resid 280 and name CA)	(segid 3A4 and resid 310 and name CB)	13.34	0.25	0.25
	assign (segid 3A4 and resid 280 and name CA)	(segid 3A4 and resid 311 and name CA)	12.65	0.28	0.28
25	assign (segid 3A4 and resid 280 and name CA)	(segid 3A4 and resid 311 and name CB)	11.64	0.32	0.33
	assign (segid 3A4 and resid 280 and name CA)	(segid 3A4 and resid 312 and name CA)	12.95	0.27	0.28
	assign (segid 3A4 and resid 280 and name CA)	(segid 3A4 and resid 312 and name CB)	12.23	0.29	0.29
	assign (segid 3A4 and resid 280 and name CA)	(segid 3A4 and resid 313 and name CA)	16.08	0.22	0.22
	assign (segid 3A4 and resid 280 and name CA)	(segid 3A4 and resid 313 and name CB)	16.29	0.22	0.21
30	assign (segid 3A4 and resid 280 and name CA)	(segid 3A4 and resid 314 and name CA)	17.38	0.27	0.26
	assign (segid 3A4 and resid 280 and name CA)	(segid 3A4 and resid 314 and name CB)	16.93	0.27	0.27
	assign (segid 3A4 and resid 280 and name CA)	(segid 3A4 and resid 315 and name CA)	17.07	0.46	0.47
	assign (segid 3A4 and resid 280 and name CA)	(segid 3A4 and resid 315 and name CB)	15.89	0.54	0.54
	assign (segid 3A4 and resid 280 and name CA)	(segid 3A4 and resid 316 and name CA)	18.36	0.40	0.41
35	assign (segid 3A4 and resid 280 and name CA)	(segid 3A4 and resid 362 and name CA)	16.90	0.56	0.55
	assign (segid 3A4 and resid 280 and name CA)	(segid 3A4 and resid 362 and name CB)	17.01	0.61	0.61
	assign (segid 3A4 and resid 280 and name CA)	(segid 3A4 and resid 363 and name CA)	13.47	0.49	0.49
	assign (segid 3A4 and resid 280 and name CA)	(segid 3A4 and resid 363 and name CB)	12.93	0.49	0.49
	assign (segid 3A4 and resid 280 and name CA)	(segid 3A4 and resid 364 and name CA)	11.80	0.58	0.58
40	assign (segid 3A4 and resid 280 and name CA)	(segid 3A4 and resid 364 and name CB)	12.96	0.63	0.63
	assign (segid 3A4 and resid 280 and name CA)	(segid 3A4 and resid 365 and name CA)	9.18	0.73	0.73
	assign (segid 3A4 and resid 280 and name CA)	(segid 3A4 and resid 365 and name CB)	7.69	0.75	0.74
	assign (segid 3A4 and resid 280 and name CA)	(segid 3A4 and resid 397 and name CA)	19.00	0.23	0.22
	assign (segid 3A4 and resid 280 and name CA)	(segid 3A4 and resid 397 and name CB)	19.49	0.28	0.27
45	assign (segid 3A4 and resid 280 and name CA)	(segid 3A4 and resid 398 and name CA)	16.06	0.30	0.31
	assign (segid 3A4 and resid 280 and name CA)	(segid 3A4 and resid 398 and name CB)	16.25	0.38	0.39
	assign (segid 3A4 and resid 280 and name CA)	(segid 3A4 and resid 399 and name CA)	16.21	0.14	0.15
	assign (segid 3A4 and resid 280 and name CA)	(segid 3A4 and resid 399 and name CB)	17.53	0.15	0.15
	assign (segid 3A4 and resid 280 and name CA)	(segid 3A4 and resid 400 and name CA)	16.40	0.14	0.15
50	assign (segid 3A4 and resid 280 and name CA)	(segid 3A4 and resid 400 and name CB)	17.57	0.18	0.17
	assign (segid 3A4 and resid 280 and name CA)	(segid 3A4 and resid 401 and name CA)	13.49	0.15	0.15
	assign (segid 3A4 and resid 280 and name CA)	(segid 3A4 and resid 402 and name CA)	11.17	0.18	0.18
	assign (segid 3A4 and resid 280 and name CA)	(segid 3A4 and resid 402 and name CB)	11.60	0.23	0.24
	assign (segid 3A4 and resid 280 and name CA)	(segid 3A4 and resid 403 and name CA)	12.81	0.20	0.20
55	assign (segid 3A4 and resid 280 and name CA)	(segid 3A4 and resid 403 and name CB)	14.33	0.20	0.20
	assign (segid 3A4 and resid 280 and name CA)	(segid 3A4 and resid 404 and name CA)	12.76	0.41	0.40
	assign (segid 3A4 and resid 280 and name CA)	(segid 3A4 and resid 404 and name CB)	13.49	0.45	0.45
	assign (segid 3A4 and resid 280 and name CA)	(segid 3A4 and resid 405 and name CA)	9.22	0.52	0.51
	assign (segid 3A4 and resid 280 and name CA)	(segid 3A4 and resid 405 and name CB)	8.61	0.45	0.46
60	assign (segid 3A4 and resid 280 and name CA)	(segid 3A4 and resid 406 and name CA)	8.34	0.46	0.46
	assign (segid 3A4 and resid 280 and name CA)	(segid 3A4 and resid 407 and name CA)	11.24	0.57	0.57
	assign (segid 3A4 and resid 280 and name CA)	(segid 3A4 and resid 407 and name CB)	12.63	0.53	0.54
	assign (segid 3A4 and resid 280 and name CA)	(segid 3A4 and resid 408 and name CA)	11.08	0.49	0.48
	assign (segid 3A4 and resid 280 and name CA)	(segid 3A4 and resid 408 and name CB)	11.12	0.52	0.52
65	assign (segid 3A4 and resid 280 and name CA)	(segid 3A4 and resid 409 and name CA)	8.07	0.50	0.50
	assign (segid 3A4 and resid 280 and name CA)	(segid 3A4 and resid 409 and name CB)	6.67	0.51	0.52
	assign (segid 3A4 and resid 280 and name CA)	(segid 3A4 and resid 410 and name CA)	9.50	0.31	0.31
	assign (segid 3A4 and resid 280 and name CA)	(segid 3A4 and resid 411 and name CA)	12.74	0.40	0.40
	assign (segid 3A4 and resid 280 and name CA)	(segid 3A4 and resid 411 and name CB)	13.61	0.36	0.36
70	assign (segid 3A4 and resid 280 and name CA)	(segid 3A4 and resid 412 and name CA)	12.43	0.60	0.60
	assign (segid 3A4 and resid 280 and name CA)	(segid 3A4 and resid 413 and name CA)	12.83	1.02	1.02
	assign (segid 3A4 and resid 280 and name CA)	(segid 3A4 and resid 414 and name CA)	13.60	1.11	1.11
	assign (segid 3A4 and resid 280 and name CA)	(segid 3A4 and resid 415 and name CA)	15.87	1.22	1.21
	assign (segid 3A4 and resid 280 and name CA)	(segid 3A4 and resid 415 and name CB)	16.58	1.13	1.12
75	assign (segid 3A4 and resid 280 and name CA)	(segid 3A4 and resid 440 and name CA)	18.54	0.40	0.40
	assign (segid 3A4 and resid 280 and name CA)	(segid 3A4 and resid 281 and name C)	5.45	0.05	0.05
	assign (segid 3A4 and resid 280 and name CB)	(segid 3A4 and resid 281 and name CB)	4.49	0.06	0.07
	assign (segid 3A4 and resid 280 and name CB)	(segid 3A4 and resid 281 and name N)	5.36	0.07	0.07
	assign (segid 3A4 and resid 280 and name CB)	(segid 3A4 and resid 281 and name O)	3.16	0.05	0.05
80	assign (segid 3A4 and resid 280 and name CB)	(segid 3A4 and resid 281 and name O)	6.35	0.07	0.07
	assign (segid 3A4 and resid 280 and name CB)	(segid 3A4 and resid 282 and name C)	6.89	0.04	0.04
	assign (segid 3A4 and resid 280 and name CB)	(segid 3A4 and resid 282 and name CA)	6.82	0.07	0.07

	assign (segid 3A4 and resid 280 and name CB)	(segid 3A4 and resid 282 and name N)	5.62	0.07	0.06
	assign (segid 3A4 and resid 280 and name CB)	(segid 3A4 and resid 303 and name CA)	8.87	0.56	0.56
	assign (segid 3A4 and resid 280 and name CB)	(segid 3A4 and resid 303 and name CB)	9.92	0.52	0.51
	assign (segid 3A4 and resid 280 and name CB)	(segid 3A4 and resid 304 and name C)	5.87	0.23	0.22
	assign (segid 3A4 and resid 280 and name CB)	(segid 3A4 and resid 304 and name CA)	6.46	0.32	0.31
5	assign (segid 3A4 and resid 280 and name CB)	(segid 3A4 and resid 304 and name CB)	5.75	0.42	0.42
	assign (segid 3A4 and resid 280 and name CB)	(segid 3A4 and resid 304 and name O)	5.99	0.29	0.29
	assign (segid 3A4 and resid 280 and name CB)	(segid 3A4 and resid 305 and name C)	6.86	0.35	0.35
	assign (segid 3A4 and resid 280 and name CB)	(segid 3A4 and resid 305 and name CA)	5.62	0.36	0.35
	assign (segid 3A4 and resid 280 and name CB)	(segid 3A4 and resid 305 and name CB)	5.88	0.52	0.51
10	assign (segid 3A4 and resid 280 and name CB)	(segid 3A4 and resid 305 and name N)	5.67	0.18	0.18
	assign (segid 3A4 and resid 280 and name CB)	(segid 3A4 and resid 305 and name O)	6.99	0.37	0.37
	assign (segid 3A4 and resid 280 and name CB)	(segid 3A4 and resid 306 and name CA)	9.24	0.31	0.31
	assign (segid 3A4 and resid 280 and name CB)	(segid 3A4 and resid 307 and name CA)	9.28	0.27	0.27
	assign (segid 3A4 and resid 280 and name CB)	(segid 3A4 and resid 307 and name CB)	9.13	0.40	0.40
15	assign (segid 3A4 and resid 280 and name CB)	(segid 3A4 and resid 308 and name CA)	7.06	0.19	0.19
	assign (segid 3A4 and resid 280 and name CB)	(segid 3A4 and resid 308 and name CB)	5.62	0.17	0.18
	assign (segid 3A4 and resid 280 and name CB)	(segid 3A4 and resid 308 and name N)	7.44	0.21	0.22
	assign (segid 3A4 and resid 280 and name CB)	(segid 3A4 and resid 309 and name CA)	9.54	0.32	0.33
	assign (segid 3A4 and resid 280 and name CB)	(segid 3A4 and resid 309 and name CB)	9.97	0.40	0.40
20	assign (segid 3A4 and resid 280 and name CB)	(segid 3A4 and resid 310 and name CA)	12.30	0.20	0.20
	assign (segid 3A4 and resid 280 and name CB)	(segid 3A4 and resid 310 and name CB)	12.65	0.21	0.21
	assign (segid 3A4 and resid 280 and name CB)	(segid 3A4 and resid 311 and name CA)	11.77	0.26	0.27
	assign (segid 3A4 and resid 280 and name CB)	(segid 3A4 and resid 311 and name CB)	10.85	0.32	0.32
	assign (segid 3A4 and resid 280 and name CB)	(segid 3A4 and resid 312 and name CA)	11.74	0.25	0.26
25	assign (segid 3A4 and resid 280 and name CB)	(segid 3A4 and resid 312 and name CB)	10.95	0.28	0.27
	assign (segid 3A4 and resid 280 and name CB)	(segid 3A4 and resid 313 and name CA)	14.91	0.23	0.22
	assign (segid 3A4 and resid 280 and name CB)	(segid 3A4 and resid 313 and name CB)	15.15	0.23	0.24
	assign (segid 3A4 and resid 280 and name CB)	(segid 3A4 and resid 314 and name CA)	16.37	0.24	0.24
	assign (segid 3A4 and resid 280 and name CB)	(segid 3A4 and resid 314 and name CB)	16.03	0.25	0.24
30	assign (segid 3A4 and resid 280 and name CB)	(segid 3A4 and resid 315 and name CA)	15.98	0.42	0.43
	assign (segid 3A4 and resid 280 and name CB)	(segid 3A4 and resid 315 and name CB)	14.81	0.50	0.51
	assign (segid 3A4 and resid 280 and name CB)	(segid 3A4 and resid 316 and name CA)	17.08	0.39	0.40
	assign (segid 3A4 and resid 280 and name CB)	(segid 3A4 and resid 362 and name CA)	16.26	0.55	0.55
35	assign (segid 3A4 and resid 280 and name CB)	(segid 3A4 and resid 362 and name CB)	16.50	0.61	0.62
	assign (segid 3A4 and resid 280 and name CB)	(segid 3A4 and resid 363 and name CA)	12.72	0.50	0.49
	assign (segid 3A4 and resid 280 and name CB)	(segid 3A4 and resid 363 and name CB)	12.06	0.50	0.51
	assign (segid 3A4 and resid 280 and name CB)	(segid 3A4 and resid 364 and name CA)	11.40	0.59	0.58
	assign (segid 3A4 and resid 280 and name CB)	(segid 3A4 and resid 364 and name CB)	12.67	0.63	0.62
40	assign (segid 3A4 and resid 280 and name CB)	(segid 3A4 and resid 365 and name CA)	8.84	0.75	0.74
	assign (segid 3A4 and resid 280 and name CB)	(segid 3A4 and resid 365 and name CB)	7.34	0.80	0.79
	assign (segid 3A4 and resid 280 and name CB)	(segid 3A4 and resid 397 and name CA)	17.90	0.23	0.24
	assign (segid 3A4 and resid 280 and name CB)	(segid 3A4 and resid 397 and name CB)	18.36	0.27	0.27
	assign (segid 3A4 and resid 280 and name CB)	(segid 3A4 and resid 398 and name CA)	15.12	0.31	0.31
	assign (segid 3A4 and resid 280 and name CB)	(segid 3A4 and resid 398 and name CB)	15.40	0.39	0.39
45	assign (segid 3A4 and resid 280 and name CB)	(segid 3A4 and resid 399 and name CA)	15.40	0.22	0.21
	assign (segid 3A4 and resid 280 and name CB)	(segid 3A4 and resid 399 and name CB)	16.76	0.24	0.23
	assign (segid 3A4 and resid 280 and name CB)	(segid 3A4 and resid 400 and name CA)	15.37	0.24	0.23
	assign (segid 3A4 and resid 280 and name CB)	(segid 3A4 and resid 400 and name CB)	16.46	0.25	0.26
50	assign (segid 3A4 and resid 280 and name CB)	(segid 3A4 and resid 401 and name CA)	12.32	0.23	0.22
	assign (segid 3A4 and resid 280 and name CB)	(segid 3A4 and resid 402 and name CA)	10.28	0.27	0.27
	assign (segid 3A4 and resid 280 and name CB)	(segid 3A4 and resid 402 and name CB)	10.85	0.31	0.31
	assign (segid 3A4 and resid 280 and name CB)	(segid 3A4 and resid 403 and name CA)	12.03	0.28	0.27
	assign (segid 3A4 and resid 280 and name CB)	(segid 3A4 and resid 403 and name CB)	13.55	0.27	0.28
55	assign (segid 3A4 and resid 280 and name CB)	(segid 3A4 and resid 404 and name CA)	11.68	0.43	0.43
	assign (segid 3A4 and resid 280 and name CB)	(segid 3A4 and resid 404 and name CB)	12.31	0.47	0.48
	assign (segid 3A4 and resid 280 and name CB)	(segid 3A4 and resid 405 and name CA)	8.05	0.50	0.49
	assign (segid 3A4 and resid 280 and name CB)	(segid 3A4 and resid 405 and name CB)	7.36	0.45	0.45
	assign (segid 3A4 and resid 280 and name CB)	(segid 3A4 and resid 405 and name O)	6.95	0.69	0.69
	assign (segid 3A4 and resid 280 and name CB)	(segid 3A4 and resid 406 and name CA)	7.70	0.50	0.49
60	assign (segid 3A4 and resid 280 and name CB)	(segid 3A4 and resid 407 and name CA)	10.60	0.53	0.54
	assign (segid 3A4 and resid 280 and name CB)	(segid 3A4 and resid 407 and name CB)	11.96	0.50	0.49
	assign (segid 3A4 and resid 280 and name CB)	(segid 3A4 and resid 408 and name CA)	10.16	0.40	0.41
	assign (segid 3A4 and resid 280 and name CB)	(segid 3A4 and resid 408 and name CB)	10.05	0.44	0.44
	assign (segid 3A4 and resid 280 and name CB)	(segid 3A4 and resid 409 and name CA)	7.39	0.44	0.44
65	assign (segid 3A4 and resid 280 and name CB)	(segid 3A4 and resid 409 and name CB)	5.95	0.45	0.46
	assign (segid 3A4 and resid 280 and name CB)	(segid 3A4 and resid 409 and name CD2)	6.26	0.72	0.72
	assign (segid 3A4 and resid 280 and name CB)	(segid 3A4 and resid 409 and name CG)	5.67	0.62	0.62
	assign (segid 3A4 and resid 280 and name CB)	(segid 3A4 and resid 410 and name CA)	9.33	0.30	0.31
	assign (segid 3A4 and resid 280 and name CB)	(segid 3A4 and resid 411 and name CA)	12.36	0.37	0.38
70	assign (segid 3A4 and resid 280 and name CB)	(segid 3A4 and resid 411 and name CB)	13.12	0.35	0.34
	assign (segid 3A4 and resid 280 and name CB)	(segid 3A4 and resid 412 and name CA)	11.89	0.60	0.60
	assign (segid 3A4 and resid 280 and name CB)	(segid 3A4 and resid 413 and name CA)	12.33	1.02	1.02
	assign (segid 3A4 and resid 280 and name CB)	(segid 3A4 and resid 414 and name CA)	12.76	1.16	1.16
	assign (segid 3A4 and resid 280 and name CB)	(segid 3A4 and resid 415 and name CA)	14.97	1.23	1.22
75	assign (segid 3A4 and resid 280 and name CB)	(segid 3A4 and resid 415 and name CB)	15.74	1.09	1.10
	assign (segid 3A4 and resid 280 and name CB)	(segid 3A4 and resid 440 and name CA)	17.39	0.42	0.42
	assign (segid 3A4 and resid 280 and name CB)	(segid 3A4 and resid 280 and name C)	2.46	0.03	0.02
	assign (segid 3A4 and resid 280 and name N)	(segid 3A4 and resid 280 and name CA)	1.46	0.01	0.01
	assign (segid 3A4 and resid 280 and name N)	(segid 3A4 and resid 280 and name CB)	2.46	0.03	0.03
80	assign (segid 3A4 and resid 280 and name N)	(segid 3A4 and resid 280 and name O)	3.51	0.05	0.04
	assign (segid 3A4 and resid 280 and name N)	(segid 3A4 and resid 281 and name C)	4.72	0.05	0.04
	assign (segid 3A4 and resid 280 and name N)	(segid 3A4 and resid 281 and name CA)	4.21	0.04	0.04

	assign (segid 3A4 and resid 280 and name N)	(segid 3A4 and resid 281 and name CB)	4.96	0.07	0.06
	assign (segid 3A4 and resid 280 and name N)	(segid 3A4 and resid 281 and name N)	2.80	0.05	0.05
	assign (segid 3A4 and resid 280 and name N)	(segid 3A4 and resid 281 and name O)	5.83	0.06	0.07
	assign (segid 3A4 and resid 280 and name N)	(segid 3A4 and resid 282 and name C)	5.61	0.08	0.07
5	assign (segid 3A4 and resid 280 and name N)	(segid 3A4 and resid 282 and name CA)	5.32	0.08	0.08
	assign (segid 3A4 and resid 280 and name N)	(segid 3A4 and resid 282 and name N)	4.31	0.06	0.05
	assign (segid 3A4 and resid 280 and name N)	(segid 3A4 and resid 282 and name O)	6.80	0.09	0.08
	assign (segid 3A4 and resid 280 and name N)	(segid 3A4 and resid 304 and name C)	6.64	0.24	0.24
	assign (segid 3A4 and resid 280 and name N)	(segid 3A4 and resid 304 and name CA)	6.70	0.22	0.22
	assign (segid 3A4 and resid 280 and name N)	(segid 3A4 and resid 304 and name CB)	5.56	0.30	0.29
10	assign (segid 3A4 and resid 280 and name N)	(segid 3A4 and resid 304 and name N)	7.25	0.35	0.34
	assign (segid 3A4 and resid 280 and name N)	(segid 3A4 and resid 304 and name O)	6.85	0.31	0.31
	assign (segid 3A4 and resid 280 and name N)	(segid 3A4 and resid 305 and name N)	6.76	0.30	0.29
	assign (segid 3A4 and resid 280 and name N)	(segid 3A4 and resid 308 and name CB)	7.15	0.17	0.17
	assign (segid 3A4 and resid 280 and name N)	(segid 3A4 and resid 308 and name N)	3.26	0.05	0.05
15	assign (segid 3A4 and resid 280 and name O)	(segid 3A4 and resid 281 and name C)	3.04	0.07	0.07
	assign (segid 3A4 and resid 280 and name O)	(segid 3A4 and resid 281 and name CA)	2.78	0.03	0.02
	assign (segid 3A4 and resid 280 and name O)	(segid 3A4 and resid 281 and name CB)	4.26	0.02	0.03
	assign (segid 3A4 and resid 280 and name O)	(segid 3A4 and resid 281 and name N)	2.25	0.02	0.02
	assign (segid 3A4 and resid 280 and name O)	(segid 3A4 and resid 281 and name O)	3.56	0.10	0.11
20	assign (segid 3A4 and resid 280 and name O)	(segid 3A4 and resid 282 and name C)	4.19	0.18	0.17
	assign (segid 3A4 and resid 280 and name O)	(segid 3A4 and resid 282 and name CA)	4.45	0.14	0.13
	assign (segid 3A4 and resid 280 and name O)	(segid 3A4 and resid 282 and name N)	3.48	0.12	0.13
	assign (segid 3A4 and resid 280 and name O)	(segid 3A4 and resid 282 and name O)	5.12	0.22	0.21
	assign (segid 3A4 and resid 280 and name O)	(segid 3A4 and resid 304 and name C)	6.44	0.33	0.32
25	assign (segid 3A4 and resid 280 and name O)	(segid 3A4 and resid 304 and name CA)	6.57	0.49	0.49
	assign (segid 3A4 and resid 280 and name O)	(segid 3A4 and resid 304 and name CB)	5.95	0.48	0.47
	assign (segid 3A4 and resid 280 and name O)	(segid 3A4 and resid 304 and name N)	7.13	0.33	0.34
	assign (segid 3A4 and resid 280 and name O)	(segid 3A4 and resid 305 and name CA)	6.29	0.33	0.34
	assign (segid 3A4 and resid 280 and name O)	(segid 3A4 and resid 305 and name CB)	6.05	0.51	0.52
30	assign (segid 3A4 and resid 280 and name O)	(segid 3A4 and resid 305 and name N)	5.94	0.24	0.24
	assign (segid 3A4 and resid 280 and name O)	(segid 3A4 and resid 409 and name CB)	6.12	0.73	0.73
	assign (segid 3A4 and resid 280 and name O)	(segid 3A4 and resid 281 and name CB)	2.48	0.04	0.05
	assign (segid 3A4 and resid 281 and name C)	(segid 3A4 and resid 281 and name O)	1.24	0.01	0.01
	assign (segid 3A4 and resid 281 and name C)	(segid 3A4 and resid 282 and name C)	3.06	0.12	0.11
35	assign (segid 3A4 and resid 281 and name C)	(segid 3A4 and resid 282 and name CA)	2.42	0.01	0.02
	assign (segid 3A4 and resid 281 and name C)	(segid 3A4 and resid 282 and name N)	1.33	0.00	0.00
	assign (segid 3A4 and resid 281 and name C)	(segid 3A4 and resid 282 and name O)	3.92	0.22	0.22
	assign (segid 3A4 and resid 281 and name C)	(segid 3A4 and resid 281 and name C)	1.51	0.01	0.02
	assign (segid 3A4 and resid 281 and name CA)	(segid 3A4 and resid 281 and name CB)	1.53	0.02	0.02
40	assign (segid 3A4 and resid 281 and name CA)	(segid 3A4 and resid 281 and name O)	2.39	0.03	0.02
	assign (segid 3A4 and resid 281 and name CA)	(segid 3A4 and resid 282 and name C)	4.42	0.11	0.11
	assign (segid 3A4 and resid 281 and name CA)	(segid 3A4 and resid 282 and name CA)	3.79	0.01	0.01
	assign (segid 3A4 and resid 281 and name CA)	(segid 3A4 and resid 282 and name N)	2.42	0.00	0.00
	assign (segid 3A4 and resid 281 and name CA)	(segid 3A4 and resid 282 and name O)	5.35	0.22	0.22
45	assign (segid 3A4 and resid 281 and name CA)	(segid 3A4 and resid 303 and name CA)	10.32	1.05	1.06
	assign (segid 3A4 and resid 281 and name CA)	(segid 3A4 and resid 303 and name CB)	11.12	1.03	1.03
	assign (segid 3A4 and resid 281 and name CA)	(segid 3A4 and resid 304 and name CA)	9.19	0.41	0.40
	assign (segid 3A4 and resid 281 and name CA)	(segid 3A4 and resid 304 and name CB)	8.38	0.38	0.39
	assign (segid 3A4 and resid 281 and name CA)	(segid 3A4 and resid 305 and name CA)	8.84	0.34	0.33
50	assign (segid 3A4 and resid 281 and name CA)	(segid 3A4 and resid 305 and name CB)	8.53	0.47	0.47
	assign (segid 3A4 and resid 281 and name CA)	(segid 3A4 and resid 306 and name CA)	12.63	0.33	0.33
	assign (segid 3A4 and resid 281 and name CA)	(segid 3A4 and resid 307 and name CA)	13.21	0.30	0.29
	assign (segid 3A4 and resid 281 and name CA)	(segid 3A4 and resid 307 and name CB)	12.90	0.38	0.38
	assign (segid 3A4 and resid 281 and name CA)	(segid 3A4 and resid 308 and name CA)	11.44	0.22	0.22
55	assign (segid 3A4 and resid 281 and name CA)	(segid 3A4 and resid 308 and name CB)	10.00	0.21	0.21
	assign (segid 3A4 and resid 281 and name CA)	(segid 3A4 and resid 309 and name CA)	13.69	0.28	0.28
	assign (segid 3A4 and resid 281 and name CA)	(segid 3A4 and resid 309 and name CB)	13.86	0.35	0.35
	assign (segid 3A4 and resid 281 and name CA)	(segid 3A4 and resid 310 and name CA)	16.59	0.23	0.23
	assign (segid 3A4 and resid 281 and name CA)	(segid 3A4 and resid 310 and name CB)	16.86	0.25	0.26
60	assign (segid 3A4 and resid 281 and name CA)	(segid 3A4 and resid 311 and name CA)	16.24	0.27	0.27
	assign (segid 3A4 and resid 281 and name CA)	(segid 3A4 and resid 311 and name CB)	15.29	0.31	0.31
	assign (segid 3A4 and resid 281 and name CA)	(segid 3A4 and resid 312 and name CA)	16.10	0.20	0.19
	assign (segid 3A4 and resid 281 and name CA)	(segid 3A4 and resid 312 and name CB)	15.20	0.17	0.16
	assign (segid 3A4 and resid 281 and name CA)	(segid 3A4 and resid 313 and name CA)	19.23	0.15	0.16
65	assign (segid 3A4 and resid 281 and name CA)	(segid 3A4 and resid 313 and name CB)	19.44	0.17	0.16
	assign (segid 3A4 and resid 281 and name CA)	(segid 3A4 and resid 315 and name CB)	19.13	0.46	0.45
	assign (segid 3A4 and resid 281 and name CA)	(segid 3A4 and resid 363 and name CA)	16.70	0.50	0.51
	assign (segid 3A4 and resid 281 and name CA)	(segid 3A4 and resid 363 and name CB)	16.00	0.51	0.50
	assign (segid 3A4 and resid 281 and name CA)	(segid 3A4 and resid 364 and name CA)	15.29	0.57	0.57
70	assign (segid 3A4 and resid 281 and name CA)	(segid 3A4 and resid 364 and name CB)	16.43	0.62	0.62
	assign (segid 3A4 and resid 281 and name CA)	(segid 3A4 and resid 365 and name CA)	12.92	0.72	0.72
	assign (segid 3A4 and resid 281 and name CA)	(segid 3A4 and resid 365 and name CB)	11.42	0.74	0.74
	assign (segid 3A4 and resid 281 and name CA)	(segid 3A4 and resid 398 and name CA)	18.32	0.38	0.38
	assign (segid 3A4 and resid 281 and name CA)	(segid 3A4 and resid 398 and name CB)	18.68	0.44	0.43
75	assign (segid 3A4 and resid 281 and name CA)	(segid 3A4 and resid 399 and name CA)	17.80	0.26	0.26
	assign (segid 3A4 and resid 281 and name CA)	(segid 3A4 and resid 399 and name CB)	19.00	0.27	0.27
	assign (segid 3A4 and resid 281 and name CA)	(segid 3A4 and resid 400 and name CA)	17.62	0.21	0.21
	assign (segid 3A4 and resid 281 and name CA)	(segid 3A4 and resid 400 and name CB)	18.82	0.21	0.21
	assign (segid 3A4 and resid 281 and name CA)	(segid 3A4 and resid 401 and name CA)	15.14	0.19	0.20
80	assign (segid 3A4 and resid 281 and name CA)	(segid 3A4 and resid 402 and name CA)	12.75	0.28	0.28
	assign (segid 3A4 and resid 281 and name CA)	(segid 3A4 and resid 402 and name CB)	13.32	0.35	0.36
	assign (segid 3A4 and resid 281 and name CA)	(segid 3A4 and resid 403 and name CA)	13.35	0.21	0.21

	assign (segid 3A4 and resid 281 and name CA) (segid 3A4 and resid 403 and name CB)	14.79	0.21	0.21
	assign (segid 3A4 and resid 281 and name CA) (segid 3A4 and resid 404 and name CA)	13.06	0.32	0.33
	assign (segid 3A4 and resid 281 and name CA) (segid 3A4 and resid 404 and name CB)	11.03	0.35	0.34
	assign (segid 3A4 and resid 281 and name CA) (segid 3A4 and resid 405 and name CA)	9.89	0.40	0.40
5	assign (segid 3A4 and resid 281 and name CA) (segid 3A4 and resid 405 and name CB)	9.85	0.38	0.38
	assign (segid 3A4 and resid 281 and name CA) (segid 3A4 and resid 406 and name CA)	8.26	0.31	0.30
	assign (segid 3A4 and resid 281 and name CA) (segid 3A4 and resid 407 and name CA)	10.10	0.52	0.52
	assign (segid 3A4 and resid 281 and name CA) (segid 3A4 and resid 407 and name CB)	11.60	0.49	0.50
	assign (segid 3A4 and resid 281 and name CA) (segid 3A4 and resid 408 and name CA)	9.90	0.60	0.60
10	assign (segid 3A4 and resid 281 and name CA) (segid 3A4 and resid 408 and name CB)	10.37	0.64	0.64
	assign (segid 3A4 and resid 281 and name CA) (segid 3A4 and resid 409 and name C)	6.02	0.60	0.60
	assign (segid 3A4 and resid 281 and name CA) (segid 3A4 and resid 409 and name N)	6.37	0.65	0.65
	assign (segid 3A4 and resid 281 and name CA) (segid 3A4 and resid 409 and name CB)	5.38	0.66	0.65
	assign (segid 3A4 and resid 281 and name CA) (segid 3A4 and resid 409 and name CG)	6.13	0.70	0.70
15	assign (segid 3A4 and resid 281 and name CA) (segid 3A4 and resid 409 and name O)	5.66	0.67	0.67
	assign (segid 3A4 and resid 281 and name CA) (segid 3A4 and resid 410 and name CA)	6.79	0.42	0.41
	assign (segid 3A4 and resid 281 and name CA) (segid 3A4 and resid 410 and name N)	6.54	0.49	0.49
	assign (segid 3A4 and resid 281 and name CA) (segid 3A4 and resid 411 and name CA)	10.04	0.55	0.55
	assign (segid 3A4 and resid 281 and name CA) (segid 3A4 and resid 411 and name CB)	11.16	0.51	0.51
20	assign (segid 3A4 and resid 281 and name CA) (segid 3A4 and resid 412 and name CA)	9.94	0.66	0.65
	assign (segid 3A4 and resid 281 and name CA) (segid 3A4 and resid 413 and name CA)	10.72	1.36	1.36
	assign (segid 3A4 and resid 281 and name CA) (segid 3A4 and resid 414 and name CA)	12.36	1.54	1.54
	assign (segid 3A4 and resid 281 and name CA) (segid 3A4 and resid 415 and name CA)	15.09	1.69	1.70
	assign (segid 3A4 and resid 281 and name CA) (segid 3A4 and resid 415 and name CB)	15.69	1.71	1.71
25	assign (segid 3A4 and resid 281 and name CA) (segid 3A4 and resid 440 and name CA)	17.90	0.71	0.71
	assign (segid 3A4 and resid 281 and name CB) (segid 3A4 and resid 282 and name C)	5.44	0.11	0.11
	assign (segid 3A4 and resid 281 and name CB) (segid 3A4 and resid 282 and name CA)	4.47	0.04	0.03
	assign (segid 3A4 and resid 281 and name CB) (segid 3A4 and resid 282 and name N)	3.15	0.03	0.04
	assign (segid 3A4 and resid 281 and name CB) (segid 3A4 and resid 282 and name O)	6.33	0.22	0.22
30	assign (segid 3A4 and resid 281 and name CB) (segid 3A4 and resid 303 and name CA)	11.83	1.02	1.02
	assign (segid 3A4 and resid 281 and name CB) (segid 3A4 and resid 303 and name CB)	12.61	0.99	0.99
	assign (segid 3A4 and resid 281 and name CB) (segid 3A4 and resid 304 and name CA)	10.56	0.36	0.36
	assign (segid 3A4 and resid 281 and name CB) (segid 3A4 and resid 304 and name CB)	9.69	0.36	0.35
35	assign (segid 3A4 and resid 281 and name CB) (segid 3A4 and resid 305 and name CA)	10.14	0.36	0.35
	assign (segid 3A4 and resid 281 and name CB) (segid 3A4 and resid 305 and name CB)	9.85	0.47	0.47
	assign (segid 3A4 and resid 281 and name CB) (segid 3A4 and resid 306 and name CA)	13.95	0.34	0.34
	assign (segid 3A4 and resid 281 and name CB) (segid 3A4 and resid 307 and name CA)	14.41	0.29	0.28
	assign (segid 3A4 and resid 281 and name CB) (segid 3A4 and resid 307 and name CB)	14.11	0.38	0.37
40	assign (segid 3A4 and resid 281 and name CB) (segid 3A4 and resid 308 and name CA)	12.38	0.22	0.22
	assign (segid 3A4 and resid 281 and name CB) (segid 3A4 and resid 308 and name CB)	10.92	0.22	0.21
	assign (segid 3A4 and resid 281 and name CB) (segid 3A4 and resid 309 and name CA)	14.63	0.32	0.32
	assign (segid 3A4 and resid 281 and name CB) (segid 3A4 and resid 309 and name CB)	14.88	0.39	0.39
	assign (segid 3A4 and resid 281 and name CB) (segid 3A4 and resid 310 and name CA)	17.60	0.25	0.25
45	assign (segid 3A4 and resid 281 and name CB) (segid 3A4 and resid 310 and name CB)	17.95	0.27	0.28
	assign (segid 3A4 and resid 281 and name CB) (segid 3A4 and resid 311 and name CA)	17.03	0.25	0.25
	assign (segid 3A4 and resid 281 and name CB) (segid 3A4 and resid 311 and name CB)	16.05	0.28	0.29
	assign (segid 3A4 and resid 281 and name CB) (segid 3A4 and resid 312 and name CA)	16.69	0.19	0.19
	assign (segid 3A4 and resid 281 and name CB) (segid 3A4 and resid 312 and name CB)	15.78	0.18	0.18
50	assign (segid 3A4 and resid 281 and name CB) (segid 3A4 and resid 363 and name CA)	16.98	0.50	0.50
	assign (segid 3A4 and resid 281 and name CB) (segid 3A4 and resid 363 and name CB)	16.20	0.51	0.50
	assign (segid 3A4 and resid 281 and name CB) (segid 3A4 and resid 364 and name CA)	15.78	0.56	0.56
	assign (segid 3A4 and resid 281 and name CB) (segid 3A4 and resid 364 and name CB)	16.92	0.61	0.61
	assign (segid 3A4 and resid 281 and name CB) (segid 3A4 and resid 365 and name CA)	13.70	0.70	0.71
	assign (segid 3A4 and resid 281 and name CB) (segid 3A4 and resid 365 and name CB)	12.21	0.73	0.74
55	assign (segid 3A4 and resid 281 and name CB) (segid 3A4 and resid 399 and name CA)	18.90	0.28	0.29
	assign (segid 3A4 and resid 281 and name CB) (segid 3A4 and resid 400 and name CA)	18.48	0.23	0.23
	assign (segid 3A4 and resid 281 and name CB) (segid 3A4 and resid 400 and name CB)	19.62	0.22	0.22
	assign (segid 3A4 and resid 281 and name CB) (segid 3A4 and resid 401 and name CA)	15.96	0.19	0.20
60	assign (segid 3A4 and resid 281 and name CB) (segid 3A4 and resid 402 and name CA)	13.81	0.31	0.31
	assign (segid 3A4 and resid 281 and name CB) (segid 3A4 and resid 402 and name CB)	14.48	0.37	0.38
	assign (segid 3A4 and resid 281 and name CB) (segid 3A4 and resid 403 and name CA)	14.26	0.24	0.25
	assign (segid 3A4 and resid 281 and name CB) (segid 3A4 and resid 403 and name CB)	15.69	0.24	0.25
	assign (segid 3A4 and resid 281 and name CB) (segid 3A4 and resid 404 and name CA)	13.64	0.28	0.28
65	assign (segid 3A4 and resid 281 and name CB) (segid 3A4 and resid 404 and name CB)	14.55	0.30	0.30
	assign (segid 3A4 and resid 281 and name CB) (segid 3A4 and resid 405 and name CA)	10.48	0.31	0.31
	assign (segid 3A4 and resid 281 and name CB) (segid 3A4 and resid 405 and name CB)	10.53	0.32	0.31
	assign (segid 3A4 and resid 281 and name CB) (segid 3A4 and resid 406 and name CA)	9.11	0.33	0.32
	assign (segid 3A4 and resid 281 and name CB) (segid 3A4 and resid 407 and name CA)	10.54	0.43	0.42
	assign (segid 3A4 and resid 281 and name CB) (segid 3A4 and resid 407 and name CB)	12.04	0.41	0.42
70	assign (segid 3A4 and resid 281 and name CB) (segid 3A4 and resid 408 and name CA)	9.88	0.52	0.52
	assign (segid 3A4 and resid 281 and name CB) (segid 3A4 and resid 408 and name CB)	10.34	0.55	0.55
	assign (segid 3A4 and resid 281 and name CB) (segid 3A4 and resid 409 and name C)	5.77	0.51	0.52
	assign (segid 3A4 and resid 281 and name CB) (segid 3A4 and resid 409 and name CA)	8.18	0.56	0.56
	assign (segid 3A4 and resid 281 and name CB) (segid 3A4 and resid 409 and name CB)	5.37	0.52	0.52
75	assign (segid 3A4 and resid 281 and name CB) (segid 3A4 and resid 409 and name CD2)	6.32	0.66	0.66
	assign (segid 3A4 and resid 281 and name CB) (segid 3A4 and resid 409 and name CG)	6.12	0.56	0.56
	assign (segid 3A4 and resid 281 and name CB) (segid 3A4 and resid 409 and name O)	5.16	0.60	0.59
	assign (segid 3A4 and resid 281 and name CB) (segid 3A4 and resid 410 and name CA)	6.70	0.42	0.43
	assign (segid 3A4 and resid 281 and name CB) (segid 3A4 and resid 410 and name N)	6.49	0.44	0.44
80	assign (segid 3A4 and resid 281 and name CB) (segid 3A4 and resid 411 and name CA)	9.59	0.60	0.60
	assign (segid 3A4 and resid 281 and name CB) (segid 3A4 and resid 411 and name CB)	10.80	0.54	0.54
	assign (segid 3A4 and resid 281 and name CB) (segid 3A4 and resid 412 and name CA)	9.06	0.69	0.70
	assign (segid 3A4 and resid 281 and name CB) (segid 3A4 and resid 413 and name CA)	9.45	1.37	1.37

	assign (segid 3A4 and resid 281 and name CB)	(segid 3A4 and resid 414 and name CA)	11.30	1.52	1.53
	assign (segid 3A4 and resid 281 and name CB)	(segid 3A4 and resid 415 and name CA)	14.02	1.74	1.74
	assign (segid 3A4 and resid 281 and name CB)	(segid 3A4 and resid 415 and name CB)	14.54	1.80	1.81
	assign (segid 3A4 and resid 281 and name CB)	(segid 3A4 and resid 440 and name CA)	17.04	0.69	0.69
5	assign (segid 3A4 and resid 281 and name N)	(segid 3A4 and resid 281 and name C)	2.47	0.03	0.02
	assign (segid 3A4 and resid 281 and name N)	(segid 3A4 and resid 281 and name CA)	1.46	0.01	0.02
	assign (segid 3A4 and resid 281 and name N)	(segid 3A4 and resid 281 and name CB)	2.46	0.01	0.01
	assign (segid 3A4 and resid 281 and name N)	(segid 3A4 and resid 281 and name O)	3.52	0.04	0.04
	assign (segid 3A4 and resid 281 and name N)	(segid 3A4 and resid 282 and name C)	4.69	0.08	0.08
	assign (segid 3A4 and resid 281 and name N)	(segid 3A4 and resid 282 and name CA)	4.20	0.04	0.03
10	assign (segid 3A4 and resid 281 and name N)	(segid 3A4 and resid 282 and name N)	2.80	0.03	0.03
	assign (segid 3A4 and resid 281 and name N)	(segid 3A4 and resid 282 and name O)	5.79	0.16	0.15
	assign (segid 3A4 and resid 281 and name N)	(segid 3A4 and resid 304 and name CB)	7.28	0.36	0.37
	assign (segid 3A4 and resid 281 and name N)	(segid 3A4 and resid 409 and name C)	6.74	0.50	0.50
15	assign (segid 3A4 and resid 281 and name N)	(segid 3A4 and resid 409 and name CB)	5.59	0.55	0.55
	assign (segid 3A4 and resid 281 and name N)	(segid 3A4 and resid 409 and name CD2)	6.49	0.71	0.71
	assign (segid 3A4 and resid 281 and name N)	(segid 3A4 and resid 409 and name CG)	6.00	0.63	0.64
	assign (segid 3A4 and resid 281 and name N)	(segid 3A4 and resid 409 and name O)	6.51	0.57	0.57
	assign (segid 3A4 and resid 281 and name O)	(segid 3A4 and resid 281 and name CB)	3.25	0.08	0.08
20	assign (segid 3A4 and resid 281 and name O)	(segid 3A4 and resid 282 and name C)	3.08	0.15	0.16
	assign (segid 3A4 and resid 281 and name O)	(segid 3A4 and resid 282 and name CA)	2.76	0.03	0.04
	assign (segid 3A4 and resid 281 and name O)	(segid 3A4 and resid 282 and name N)	2.25	0.01	0.01
	assign (segid 3A4 and resid 281 and name O)	(segid 3A4 and resid 282 and name O)	3.59	0.31	0.31
	assign (segid 3A4 and resid 282 and name C)	(segid 3A4 and resid 282 and name O)	1.23	0.00	0.00
25	assign (segid 3A4 and resid 282 and name CA)	(segid 3A4 and resid 282 and name C)	1.51	0.00	0.01
	assign (segid 3A4 and resid 282 and name CA)	(segid 3A4 and resid 282 and name O)	2.39	0.02	0.01
	assign (segid 3A4 and resid 282 and name CA)	(segid 3A4 and resid 303 and name CA)	9.89	1.11	1.12
	assign (segid 3A4 and resid 282 and name CA)	(segid 3A4 and resid 303 and name CB)	10.19	1.13	1.12
	assign (segid 3A4 and resid 282 and name CA)	(segid 3A4 and resid 304 and name CA)	9.22	0.36	0.35
	assign (segid 3A4 and resid 282 and name CA)	(segid 3A4 and resid 304 and name CB)	8.20	0.27	0.28
30	assign (segid 3A4 and resid 282 and name CA)	(segid 3A4 and resid 305 and name CA)	10.26	0.35	0.36
	assign (segid 3A4 and resid 282 and name CA)	(segid 3A4 and resid 305 and name CB)	10.18	0.51	0.51
	assign (segid 3A4 and resid 282 and name CA)	(segid 3A4 and resid 306 and name CA)	13.78	0.28	0.28
	assign (segid 3A4 and resid 282 and name CA)	(segid 3A4 and resid 307 and name CA)	13.99	0.21	0.21
35	assign (segid 3A4 and resid 282 and name CA)	(segid 3A4 and resid 307 and name CB)	13.32	0.30	0.31
	assign (segid 3A4 and resid 282 and name CA)	(segid 3A4 and resid 308 and name CA)	13.05	0.13	0.14
	assign (segid 3A4 and resid 282 and name CA)	(segid 3A4 and resid 308 and name CB)	11.83	0.16	0.15
	assign (segid 3A4 and resid 282 and name CA)	(segid 3A4 and resid 309 and name CA)	15.78	0.24	0.23
	assign (segid 3A4 and resid 282 and name CA)	(segid 3A4 and resid 309 and name CB)	15.95	0.28	0.29
40	assign (segid 3A4 and resid 282 and name CA)	(segid 3A4 and resid 310 and name CA)	18.14	0.17	0.17
	assign (segid 3A4 and resid 282 and name CA)	(segid 3A4 and resid 310 and name CB)	18.12	0.18	0.18
	assign (segid 3A4 and resid 282 and name CA)	(segid 3A4 and resid 311 and name CA)	17.79	0.28	0.28
	assign (segid 3A4 and resid 282 and name CA)	(segid 3A4 and resid 311 and name CB)	16.69	0.32	0.32
	assign (segid 3A4 and resid 282 and name CA)	(segid 3A4 and resid 312 and name CA)	18.37	0.26	0.25
	assign (segid 3A4 and resid 282 and name CA)	(segid 3A4 and resid 312 and name CB)	17.67	0.25	0.25
45	assign (segid 3A4 and resid 282 and name CA)	(segid 3A4 and resid 312 and name CB)	18.12	0.50	0.50
	assign (segid 3A4 and resid 282 and name CA)	(segid 3A4 and resid 363 and name CA)	17.68	0.49	0.48
	assign (segid 3A4 and resid 282 and name CA)	(segid 3A4 and resid 363 and name CB)	16.03	0.59	0.58
	assign (segid 3A4 and resid 282 and name CA)	(segid 3A4 and resid 364 and name CA)	16.92	0.65	0.65
	assign (segid 3A4 and resid 282 and name CA)	(segid 3A4 and resid 364 and name CB)	13.63	0.70	0.70
50	assign (segid 3A4 and resid 282 and name CA)	(segid 3A4 and resid 365 and name CA)	12.24	0.66	0.67
	assign (segid 3A4 and resid 282 and name CA)	(segid 3A4 and resid 365 and name CB)	17.94	0.24	0.24
	assign (segid 3A4 and resid 282 and name CA)	(segid 3A4 and resid 401 and name CA)	15.12	0.30	0.29
	assign (segid 3A4 and resid 282 and name CA)	(segid 3A4 and resid 402 and name CA)	15.37	0.34	0.33
	assign (segid 3A4 and resid 282 and name CA)	(segid 3A4 and resid 402 and name CB)	15.88	0.36	0.35
55	assign (segid 3A4 and resid 282 and name CA)	(segid 3A4 and resid 403 and name CA)	17.28	0.35	0.35
	assign (segid 3A4 and resid 282 and name CA)	(segid 3A4 and resid 403 and name CB)	16.22	0.48	0.47
	assign (segid 3A4 and resid 282 and name CA)	(segid 3A4 and resid 404 and name CA)	17.26	0.46	0.47
	assign (segid 3A4 and resid 282 and name CA)	(segid 3A4 and resid 404 and name CB)	13.14	0.54	0.54
	assign (segid 3A4 and resid 282 and name CA)	(segid 3A4 and resid 405 and name CA)	12.98	0.49	0.49
60	assign (segid 3A4 and resid 282 and name CA)	(segid 3A4 and resid 405 and name CB)	11.01	0.46	0.46
	assign (segid 3A4 and resid 282 and name CA)	(segid 3A4 and resid 406 and name CA)	13.07	0.72	0.72
	assign (segid 3A4 and resid 282 and name CA)	(segid 3A4 and resid 407 and name CA)	14.53	0.71	0.71
	assign (segid 3A4 and resid 282 and name CA)	(segid 3A4 and resid 407 and name CB)	13.45	0.73	0.72
	assign (segid 3A4 and resid 282 and name CA)	(segid 3A4 and resid 408 and name CA)	14.02	0.73	0.73
65	assign (segid 3A4 and resid 282 and name CA)	(segid 3A4 and resid 408 and name CB)	10.00	0.75	0.75
	assign (segid 3A4 and resid 282 and name CA)	(segid 3A4 and resid 409 and name CA)	9.08	0.74	0.74
	assign (segid 3A4 and resid 282 and name CA)	(segid 3A4 and resid 409 and name CB)	9.58	0.68	0.68
	assign (segid 3A4 and resid 282 and name CA)	(segid 3A4 and resid 410 and name CA)	12.95	0.74	0.75
	assign (segid 3A4 and resid 282 and name CA)	(segid 3A4 and resid 411 and name CA)	14.17	0.71	0.71
70	assign (segid 3A4 and resid 282 and name CA)	(segid 3A4 and resid 411 and name CB)	13.15	0.73	0.74
	assign (segid 3A4 and resid 282 and name CA)	(segid 3A4 and resid 412 and name CA)	13.61	1.41	1.41
	assign (segid 3A4 and resid 282 and name CA)	(segid 3A4 and resid 413 and name CA)	15.60	1.44	1.45
	assign (segid 3A4 and resid 282 and name CA)	(segid 3A4 and resid 414 and name CA)	2.44	0.06	0.05
	assign (segid 3A4 and resid 282 and name N)	(segid 3A4 and resid 282 and name C)	1.46	0.01	0.00
75	assign (segid 3A4 and resid 282 and name N)	(segid 3A4 and resid 282 and name CA)	3.49	0.09	0.09
	assign (segid 3A4 and resid 282 and name N)	(segid 3A4 and resid 29 and name O)	1.24	0.01	0.01
	assign (segid 3A4 and resid 29 and name C)	(segid 3A4 and resid 30 and name C)	3.58	0.05	0.04
	assign (segid 3A4 and resid 29 and name C)	(segid 3A4 and resid 30 and name CA)	2.42	0.02	0.03
	assign (segid 3A4 and resid 29 and name C)	(segid 3A4 and resid 30 and name N)	1.33	0.01	0.00
80	assign (segid 3A4 and resid 29 and name C)	(segid 3A4 and resid 30 and name O)	3.95	0.12	0.12
	assign (segid 3A4 and resid 29 and name C)	(segid 3A4 and resid 31 and name C)	6.74	0.11	0.11
	assign (segid 3A4 and resid 29 and name C)	(segid 3A4 and resid 31 and name CA)	5.83	0.15	0.15

	assign (segid 3A4 and resid 29 and name C) (segid 3A4 and resid 31 and name CB)	6.64	0.25	0.24
	assign (segid 3A4 and resid 29 and name C) (segid 3A4 and resid 31 and name N)	4.55	0.14	0.14
	assign (segid 3A4 and resid 29 and name C) (segid 3A4 and resid 31 and name O)	6.88	0.22	0.22
	assign (segid 3A4 and resid 29 and name C) (segid 3A4 and resid 32 and name N)	7.65	0.11	0.10
5	assign (segid 3A4 and resid 29 and name C) (segid 3A4 and resid 341 and name C)	6.67	0.47	0.48
	assign (segid 3A4 and resid 29 and name C) (segid 3A4 and resid 341 and name CA)	6.69	0.50	0.51
	assign (segid 3A4 and resid 29 and name C) (segid 3A4 and resid 341 and name CB)	6.74	0.59	0.58
	assign (segid 3A4 and resid 29 and name C) (segid 3A4 and resid 341 and name CG)	6.97	0.44	0.44
	assign (segid 3A4 and resid 29 and name C) (segid 3A4 and resid 342 and name C)	5.91	0.30	0.30
	assign (segid 3A4 and resid 29 and name C) (segid 3A4 and resid 342 and name CA)	5.95	0.37	0.37
10	assign (segid 3A4 and resid 29 and name C) (segid 3A4 and resid 342 and name N)	5.62	0.41	0.42
	assign (segid 3A4 and resid 29 and name C) (segid 3A4 and resid 342 and name O)	5.11	0.26	0.27
	assign (segid 3A4 and resid 29 and name C) (segid 3A4 and resid 343 and name CA)	7.58	0.23	0.24
	assign (segid 3A4 and resid 29 and name C) (segid 3A4 and resid 343 and name N)	7.06	0.28	0.27
	assign (segid 3A4 and resid 29 and name C) (segid 3A4 and resid 343 and name O)	1.52	0.01	0.01
15	assign (segid 3A4 and resid 29 and name CA) (segid 3A4 and resid 29 and name C)	2.41	0.03	0.02
	assign (segid 3A4 and resid 29 and name CA) (segid 3A4 and resid 30 and name C)	4.73	0.03	0.04
	assign (segid 3A4 and resid 29 and name CA) (segid 3A4 and resid 30 and name CA)	3.79	0.02	0.02
	assign (segid 3A4 and resid 29 and name CA) (segid 3A4 and resid 30 and name N)	2.43	0.03	0.02
20	assign (segid 3A4 and resid 29 and name CA) (segid 3A4 and resid 30 and name O)	4.80	0.14	0.14
	assign (segid 3A4 and resid 29 and name CA) (segid 3A4 and resid 31 and name CA)	6.95	0.20	0.20
	assign (segid 3A4 and resid 29 and name CA) (segid 3A4 and resid 31 and name CB)	7.78	0.34	0.33
	assign (segid 3A4 and resid 29 and name CA) (segid 3A4 and resid 31 and name N)	5.79	0.17	0.18
	assign (segid 3A4 and resid 29 and name CA) (segid 3A4 and resid 322 and name CA)	12.71	0.30	0.30
25	assign (segid 3A4 and resid 29 and name CA) (segid 3A4 and resid 323 and name CA)	12.88	0.33	0.33
	assign (segid 3A4 and resid 29 and name CA) (segid 3A4 and resid 323 and name CB)	13.56	0.44	0.44
	assign (segid 3A4 and resid 29 and name CA) (segid 3A4 and resid 324 and name CA)	11.69	0.46	0.46
	assign (segid 3A4 and resid 29 and name CA) (segid 3A4 and resid 324 and name CB)	11.90	0.54	0.55
	assign (segid 3A4 and resid 29 and name CA) (segid 3A4 and resid 325 and name CA)	12.90	0.44	0.44
	assign (segid 3A4 and resid 29 and name CA) (segid 3A4 and resid 325 and name CB)	12.31	0.43	0.44
30	assign (segid 3A4 and resid 29 and name CA) (segid 3A4 and resid 326 and name CA)	15.94	0.55	0.55
	assign (segid 3A4 and resid 29 and name CA) (segid 3A4 and resid 326 and name CB)	17.26	0.57	0.57
	assign (segid 3A4 and resid 29 and name CA) (segid 3A4 and resid 327 and name CA)	16.52	0.65	0.66
	assign (segid 3A4 and resid 29 and name CA) (segid 3A4 and resid 327 and name CB)	17.96	0.67	0.68
	assign (segid 3A4 and resid 29 and name CA) (segid 3A4 and resid 328 and name CA)	15.60	0.67	0.66
35	assign (segid 3A4 and resid 29 and name CA) (segid 3A4 and resid 328 and name CB)	16.17	0.66	0.66
	assign (segid 3A4 and resid 29 and name CA) (segid 3A4 and resid 329 and name CA)	16.29	0.71	0.71
	assign (segid 3A4 and resid 29 and name CA) (segid 3A4 and resid 329 and name CB)	16.10	0.83	0.82
	assign (segid 3A4 and resid 29 and name CA) (segid 3A4 and resid 32 and name CA)	9.79	0.13	0.14
	assign (segid 3A4 and resid 29 and name CA) (segid 3A4 and resid 32 and name CB)	9.90	0.23	0.23
40	assign (segid 3A4 and resid 29 and name CA) (segid 3A4 and resid 330 and name CA)	16.92	0.60	0.60
	assign (segid 3A4 and resid 29 and name CA) (segid 3A4 and resid 330 and name CB)	18.09	0.59	0.60
	assign (segid 3A4 and resid 29 and name CA) (segid 3A4 and resid 331 and name CA)	16.51	0.65	0.66
	assign (segid 3A4 and resid 29 and name CA) (segid 3A4 and resid 331 and name CB)	15.39	0.70	0.69
	assign (segid 3A4 and resid 29 and name CA) (segid 3A4 and resid 332 and name CA)	18.50	0.57	0.58
45	assign (segid 3A4 and resid 29 and name CA) (segid 3A4 and resid 335 and name CA)	14.65	0.58	0.58
	assign (segid 3A4 and resid 29 and name CA) (segid 3A4 and resid 336 and name CA)	14.02	0.63	0.63
	assign (segid 3A4 and resid 29 and name CA) (segid 3A4 and resid 336 and name CB)	14.66	0.66	0.67
	assign (segid 3A4 and resid 29 and name CA) (segid 3A4 and resid 337 and name CA)	11.45	0.74	0.73
	assign (segid 3A4 and resid 29 and name CA) (segid 3A4 and resid 337 and name CB)	11.50	0.84	0.84
50	assign (segid 3A4 and resid 29 and name CA) (segid 3A4 and resid 338 and name CA)	11.51	0.68	0.68
	assign (segid 3A4 and resid 29 and name CA) (segid 3A4 and resid 338 and name CB)	10.95	0.76	0.76
	assign (segid 3A4 and resid 29 and name CA) (segid 3A4 and resid 339 and name CA)	12.86	0.65	0.65
	assign (segid 3A4 and resid 29 and name CA) (segid 3A4 and resid 339 and name CB)	14.13	0.63	0.63
	assign (segid 3A4 and resid 29 and name CA) (segid 3A4 and resid 33 and name CA)	13.24	0.14	0.14
55	assign (segid 3A4 and resid 29 and name CA) (segid 3A4 and resid 33 and name CB)	13.77	0.22	0.22
	assign (segid 3A4 and resid 29 and name CA) (segid 3A4 and resid 340 and name CA)	10.80	0.54	0.54
	assign (segid 3A4 and resid 29 and name CA) (segid 3A4 and resid 341 and name CA)	7.75	0.56	0.56
	assign (segid 3A4 and resid 29 and name CA) (segid 3A4 and resid 341 and name CB)	7.76	0.65	0.65
	assign (segid 3A4 and resid 29 and name CA) (segid 3A4 and resid 342 and name C)	7.39	0.29	0.30
60	assign (segid 3A4 and resid 29 and name CA) (segid 3A4 and resid 342 and name CA)	7.37	0.39	0.38
	assign (segid 3A4 and resid 29 and name CA) (segid 3A4 and resid 342 and name N)	6.94	0.44	0.43
	assign (segid 3A4 and resid 29 and name CA) (segid 3A4 and resid 342 and name O)	6.60	0.27	0.27
	assign (segid 3A4 and resid 29 and name CA) (segid 3A4 and resid 343 and name CA)	9.07	0.23	0.22
	assign (segid 3A4 and resid 29 and name CA) (segid 3A4 and resid 343 and name CB)	10.26	0.23	0.23
65	assign (segid 3A4 and resid 29 and name CA) (segid 3A4 and resid 344 and name CA)	10.55	0.25	0.25
	assign (segid 3A4 and resid 29 and name CA) (segid 3A4 and resid 344 and name CB)	9.92	0.29	0.30
	assign (segid 3A4 and resid 29 and name CA) (segid 3A4 and resid 345 and name CA)	14.06	0.12	0.13
	assign (segid 3A4 and resid 29 and name CA) (segid 3A4 and resid 345 and name CB)	15.05	0.18	0.17
	assign (segid 3A4 and resid 29 and name CA) (segid 3A4 and resid 346 and name CA)	15.67	0.25	0.26
70	assign (segid 3A4 and resid 29 and name CA) (segid 3A4 and resid 346 and name CB)	15.32	0.37	0.37
	assign (segid 3A4 and resid 29 and name CA) (segid 3A4 and resid 347 and name CA)	19.27	0.19	0.18
	assign (segid 3A4 and resid 29 and name CA) (segid 3A4 and resid 349 and name CB)	18.28	0.49	0.49
	assign (segid 3A4 and resid 29 and name CA) (segid 3A4 and resid 34 and name CA)	15.99	0.30	0.29
	assign (segid 3A4 and resid 29 and name CA) (segid 3A4 and resid 34 and name CB)	15.88	0.37	0.38
75	assign (segid 3A4 and resid 29 and name CA) (segid 3A4 and resid 35 and name CA)	19.11	0.22	0.23
	assign (segid 3A4 and resid 29 and name CA) (segid 3A4 and resid 38 and name CA)	18.41	0.36	0.37
	assign (segid 3A4 and resid 29 and name CA) (segid 3A4 and resid 38 and name CB)	17.34	0.38	0.38
	assign (segid 3A4 and resid 29 and name CA) (segid 3A4 and resid 39 and name CA)	18.14	0.14	0.13
80	assign (segid 3A4 and resid 29 and name CA) (segid 3A4 and resid 39 and name CB)	18.43	0.10	0.10
	assign (segid 3A4 and resid 29 and name CA) (segid 3A4 and resid 42 and name CA)	17.36	0.46	0.47
	assign (segid 3A4 and resid 29 and name CA) (segid 3A4 and resid 42 and name CB)	16.11	0.38	0.38
	assign (segid 3A4 and resid 29 and name N) (segid 3A4 and resid 29 and name C)	2.41	0.04	0.03

	assign (segid 3A4 and resid 29 and name N)	(segid 3A4 and resid 29 and name CA)	1.45	0.00	0.01
	assign (segid 3A4 and resid 29 and name N)	(segid 3A4 and resid 29 and name O)	2.79	0.08	0.07
	assign (segid 3A4 and resid 29 and name N)	(segid 3A4 and resid 30 and name C)	5.87	0.05	0.05
	assign (segid 3A4 and resid 29 and name N)	(segid 3A4 and resid 30 and name CA)	4.71	0.05	0.06
5	assign (segid 3A4 and resid 29 and name N)	(segid 3A4 and resid 30 and name N)	3.49	0.05	0.05
	assign (segid 3A4 and resid 29 and name N)	(segid 3A4 and resid 30 and name O)	6.04	0.16	0.16
	assign (segid 3A4 and resid 29 and name N)	(segid 3A4 and resid 31 and name N)	6.90	0.13	0.13
	assign (segid 3A4 and resid 29 and name N)	(segid 3A4 and resid 31 and name O)	7.30	0.27	0.27
	assign (segid 3A4 and resid 29 and name N)	(segid 3A4 and resid 31 and name CA)	4.07	0.08	0.08
	assign (segid 3A4 and resid 29 and name O)	(segid 3A4 and resid 30 and name CA)	2.75	0.02	0.02
10	assign (segid 3A4 and resid 29 and name O)	(segid 3A4 and resid 30 and name N)	2.25	0.01	0.00
	assign (segid 3A4 and resid 29 and name O)	(segid 3A4 and resid 30 and name O)	4.71	0.13	0.14
	assign (segid 3A4 and resid 29 and name O)	(segid 3A4 and resid 31 and name C)	7.08	0.12	0.11
	assign (segid 3A4 and resid 29 and name O)	(segid 3A4 and resid 31 and name CA)	6.18	0.16	0.15
15	assign (segid 3A4 and resid 29 and name O)	(segid 3A4 and resid 31 and name CB)	6.80	0.24	0.25
	assign (segid 3A4 and resid 29 and name O)	(segid 3A4 and resid 31 and name N)	4.81	0.13	0.13
	assign (segid 3A4 and resid 29 and name O)	(segid 3A4 and resid 31 and name O)	7.05	0.20	0.21
	assign (segid 3A4 and resid 29 and name O)	(segid 3A4 and resid 340 and name C)	7.34	0.45	0.44
	assign (segid 3A4 and resid 29 and name O)	(segid 3A4 and resid 340 and name O)	6.68	0.37	0.36
20	assign (segid 3A4 and resid 29 and name O)	(segid 3A4 and resid 341 and name C)	5.69	0.50	0.49
	assign (segid 3A4 and resid 29 and name O)	(segid 3A4 and resid 341 and name CA)	5.72	0.53	0.53
	assign (segid 3A4 and resid 29 and name O)	(segid 3A4 and resid 341 and name CB)	5.96	0.62	0.62
	assign (segid 3A4 and resid 29 and name O)	(segid 3A4 and resid 341 and name CG)	6.29	0.51	0.50
	assign (segid 3A4 and resid 29 and name O)	(segid 3A4 and resid 341 and name N)	7.01	0.52	0.52
	assign (segid 3A4 and resid 29 and name O)	(segid 3A4 and resid 341 and name O)	6.81	0.49	0.49
25	assign (segid 3A4 and resid 29 and name O)	(segid 3A4 and resid 342 and name C)	5.25	0.34	0.34
	assign (segid 3A4 and resid 29 and name O)	(segid 3A4 and resid 342 and name CA)	5.05	0.41	0.41
	assign (segid 3A4 and resid 29 and name O)	(segid 3A4 and resid 342 and name N)	4.63	0.44	0.44
	assign (segid 3A4 and resid 29 and name O)	(segid 3A4 and resid 342 and name O)	4.63	0.27	0.28
	assign (segid 3A4 and resid 29 and name O)	(segid 3A4 and resid 343 and name CA)	7.19	0.28	0.28
30	assign (segid 3A4 and resid 29 and name O)	(segid 3A4 and resid 343 and name N)	6.46	0.33	0.33
	assign (segid 3A4 and resid 29 and name O)	(segid 3A4 and resid 303 and name CB)	2.48	0.03	0.04
	assign (segid 3A4 and resid 29 and name O)	(segid 3A4 and resid 303 and name O)	1.24	0.01	0.00
	assign (segid 3A4 and resid 29 and name O)	(segid 3A4 and resid 304 and name C)	3.19	0.09	0.09
	assign (segid 3A4 and resid 29 and name O)	(segid 3A4 and resid 304 and name CA)	2.44	0.02	0.02
35	assign (segid 3A4 and resid 29 and name O)	(segid 3A4 and resid 304 and name CB)	3.69	0.02	0.02
	assign (segid 3A4 and resid 29 and name O)	(segid 3A4 and resid 304 and name N)	1.33	0.01	0.01
	assign (segid 3A4 and resid 29 and name O)	(segid 3A4 and resid 304 and name O)	4.20	0.21	0.20
	assign (segid 3A4 and resid 29 and name O)	(segid 3A4 and resid 305 and name C)	5.04	0.26	0.26
	assign (segid 3A4 and resid 29 and name O)	(segid 3A4 and resid 305 and name CA)	4.62	0.09	0.09
40	assign (segid 3A4 and resid 29 and name O)	(segid 3A4 and resid 305 and name CB)	5.21	0.16	0.16
	assign (segid 3A4 and resid 29 and name O)	(segid 3A4 and resid 305 and name N)	3.34	0.09	0.10
	assign (segid 3A4 and resid 29 and name O)	(segid 3A4 and resid 305 and name O)	6.14	0.31	0.31
	assign (segid 3A4 and resid 29 and name O)	(segid 3A4 and resid 306 and name C)	5.97	0.69	0.68
45	assign (segid 3A4 and resid 29 and name O)	(segid 3A4 and resid 306 and name CA)	5.48	0.58	0.57
	assign (segid 3A4 and resid 29 and name O)	(segid 3A4 and resid 306 and name N)	4.52	0.41	0.41
	assign (segid 3A4 and resid 29 and name O)	(segid 3A4 and resid 306 and name O)	7.19	0.70	0.70
	assign (segid 3A4 and resid 29 and name O)	(segid 3A4 and resid 307 and name C)	7.09	0.61	0.60
	assign (segid 3A4 and resid 29 and name O)	(segid 3A4 and resid 307 and name CA)	6.18	0.73	0.74
	assign (segid 3A4 and resid 29 and name O)	(segid 3A4 and resid 307 and name CB)	5.72	0.71	0.70
50	assign (segid 3A4 and resid 29 and name O)	(segid 3A4 and resid 307 and name N)	5.30	0.73	0.73
	assign (segid 3A4 and resid 29 and name O)	(segid 3A4 and resid 308 and name CB)	7.63	0.17	0.17
	assign (segid 3A4 and resid 29 and name O)	(segid 3A4 and resid 308 and name N)	6.76	0.45	0.45
	assign (segid 3A4 and resid 29 and name O)	(segid 3A4 and resid 303 and name C)	1.52	0.01	0.01
	assign (segid 3A4 and resid 29 and name O)	(segid 3A4 and resid 303 and name CB)	1.52	0.01	0.01
55	assign (segid 3A4 and resid 29 and name O)	(segid 3A4 and resid 303 and name O)	2.39	0.02	0.02
	assign (segid 3A4 and resid 29 and name O)	(segid 3A4 and resid 304 and name C)	4.53	0.06	0.06
	assign (segid 3A4 and resid 29 and name O)	(segid 3A4 and resid 304 and name CA)	3.81	0.01	0.00
	assign (segid 3A4 and resid 29 and name O)	(segid 3A4 and resid 304 and name CB)	4.83	0.03	0.04
	assign (segid 3A4 and resid 29 and name O)	(segid 3A4 and resid 304 and name N)	2.43	0.01	0.01
60	assign (segid 3A4 and resid 29 and name O)	(segid 3A4 and resid 304 and name O)	5.61	0.18	0.18
	assign (segid 3A4 and resid 29 and name O)	(segid 3A4 and resid 305 and name C)	6.08	0.30	0.30
	assign (segid 3A4 and resid 29 and name O)	(segid 3A4 and resid 305 and name CB)	5.57	0.11	0.11
	assign (segid 3A4 and resid 29 and name O)	(segid 3A4 and resid 305 and name N)	5.80	0.21	0.22
	assign (segid 3A4 and resid 29 and name O)	(segid 3A4 and resid 305 and name O)	1.39	0.11	0.11
65	assign (segid 3A4 and resid 29 and name O)	(segid 3A4 and resid 305 and name CA)	7.24	0.34	0.34
	assign (segid 3A4 and resid 29 and name O)	(segid 3A4 and resid 306 and name C)	6.42	0.75	0.75
	assign (segid 3A4 and resid 29 and name O)	(segid 3A4 and resid 306 and name N)	5.49	0.52	0.52
	assign (segid 3A4 and resid 29 and name O)	(segid 3A4 and resid 307 and name CA)	7.56	0.85	0.84
	assign (segid 3A4 and resid 29 and name O)	(segid 3A4 and resid 307 and name CB)	7.15	0.79	0.79
70	assign (segid 3A4 and resid 29 and name O)	(segid 3A4 and resid 307 and name N)	6.59	0.84	0.85
	assign (segid 3A4 and resid 29 and name O)	(segid 3A4 and resid 308 and name CA)	9.24	0.34	0.34
	assign (segid 3A4 and resid 29 and name O)	(segid 3A4 and resid 308 and name CB)	8.91	0.13	0.13
	assign (segid 3A4 and resid 29 and name O)	(segid 3A4 and resid 309 and name CA)	10.89	0.47	0.46
	assign (segid 3A4 and resid 29 and name O)	(segid 3A4 and resid 309 and name CB)	10.54	0.42	0.41
75	assign (segid 3A4 and resid 29 and name O)	(segid 3A4 and resid 310 and name CA)	12.06	0.97	0.97
	assign (segid 3A4 and resid 29 and name O)	(segid 3A4 and resid 310 and name CB)	11.48	1.15	1.15
	assign (segid 3A4 and resid 29 and name O)	(segid 3A4 and resid 311 and name CA)	13.44	0.74	0.74
	assign (segid 3A4 and resid 29 and name O)	(segid 3A4 and resid 311 and name CB)	12.87	0.66	0.66
	assign (segid 3A4 and resid 29 and name O)	(segid 3A4 and resid 312 and name CA)	15.04	0.44	0.45
80	assign (segid 3A4 and resid 29 and name O)	(segid 3A4 and resid 312 and name CB)	14.58	0.32	0.32
	assign (segid 3A4 and resid 29 and name O)	(segid 3A4 and resid 313 and name CA)	16.71	0.71	0.71
	assign (segid 3A4 and resid 29 and name O)	(segid 3A4 and resid 313 and name CB)	16.22	0.78	0.78

	assign (segid 3A4 and resid 303 and name CA)	(segid 3A4 and resid 314 and name CA)	17.87	0.90	0.90
	assign (segid 3A4 and resid 303 and name CA)	(segid 3A4 and resid 314 and name CB)	17.22	0.97	0.96
	assign (segid 3A4 and resid 303 and name CA)	(segid 3A4 and resid 315 and name CA)	19.21	0.62	0.63
	assign (segid 3A4 and resid 303 and name CA)	(segid 3A4 and resid 315 and name CB)	18.51	0.54	0.55
5	assign (segid 3A4 and resid 303 and name CA)	(segid 3A4 and resid 363 and name CA)	17.20	0.47	0.47
	assign (segid 3A4 and resid 303 and name CA)	(segid 3A4 and resid 363 and name CB)	17.20	0.41	0.41
	assign (segid 3A4 and resid 303 and name CA)	(segid 3A4 and resid 364 and name CA)	14.62	0.43	0.44
	assign (segid 3A4 and resid 303 and name CA)	(segid 3A4 and resid 364 and name CB)	15.44	0.48	0.48
	assign (segid 3A4 and resid 303 and name CA)	(segid 3A4 and resid 365 and name CA)	10.91	0.47	0.48
	assign (segid 3A4 and resid 303 and name CA)	(segid 3A4 and resid 365 and name CB)	10.02	0.42	0.41
10	assign (segid 3A4 and resid 303 and name CA)	(segid 3A4 and resid 395 and name CA)	17.06	0.98	0.98
	assign (segid 3A4 and resid 303 and name CA)	(segid 3A4 and resid 396 and name CA)	18.20	0.81	0.82
	assign (segid 3A4 and resid 303 and name CA)	(segid 3A4 and resid 397 and name CA)	17.42	0.81	0.81
	assign (segid 3A4 and resid 303 and name CA)	(segid 3A4 and resid 397 and name CB)	18.04	0.83	0.82
	assign (segid 3A4 and resid 303 and name CA)	(segid 3A4 and resid 398 and name CA)	13.76	0.84	0.84
15	assign (segid 3A4 and resid 303 and name CA)	(segid 3A4 and resid 398 and name CB)	13.33	0.89	0.88
	assign (segid 3A4 and resid 303 and name CA)	(segid 3A4 and resid 399 and name CA)	13.54	0.87	0.87
	assign (segid 3A4 and resid 303 and name CA)	(segid 3A4 and resid 399 and name CB)	14.52	0.87	0.88
	assign (segid 3A4 and resid 303 and name CA)	(segid 3A4 and resid 400 and name CA)	15.52	0.86	0.87
	assign (segid 3A4 and resid 303 and name CA)	(segid 3A4 and resid 400 and name CB)	16.89	0.85	0.86
20	assign (segid 3A4 and resid 303 and name CA)	(segid 3A4 and resid 401 and name CA)	13.67	0.65	0.65
	assign (segid 3A4 and resid 303 and name CA)	(segid 3A4 and resid 402 and name CA)	10.27	0.75	0.75
	assign (segid 3A4 and resid 303 and name CA)	(segid 3A4 and resid 402 and name CB)	9.58	0.75	0.74
	assign (segid 3A4 and resid 303 and name CA)	(segid 3A4 and resid 403 and name CA)	12.24	1.01	1.02
	assign (segid 3A4 and resid 303 and name CA)	(segid 3A4 and resid 403 and name CB)	13.39	0.97	0.98
25	assign (segid 3A4 and resid 303 and name CA)	(segid 3A4 and resid 404 and name CA)	14.37	1.14	1.14
	assign (segid 3A4 and resid 303 and name CA)	(segid 3A4 and resid 404 and name CB)	15.29	1.08	1.07
	assign (segid 3A4 and resid 303 and name CA)	(segid 3A4 and resid 405 and name CA)	12.09	1.23	1.24
	assign (segid 3A4 and resid 303 and name CA)	(segid 3A4 and resid 405 and name CB)	11.41	1.00	1.00
	assign (segid 3A4 and resid 303 and name CA)	(segid 3A4 and resid 406 and name CA)	10.08	1.39	1.39
30	assign (segid 3A4 and resid 303 and name CA)	(segid 3A4 and resid 407 and name CA)	13.60	1.42	1.42
	assign (segid 3A4 and resid 303 and name CA)	(segid 3A4 and resid 407 and name CB)	14.53	1.41	1.42
	assign (segid 3A4 and resid 303 and name CA)	(segid 3A4 and resid 408 and name CA)	15.43	1.30	1.29
	assign (segid 3A4 and resid 303 and name CA)	(segid 3A4 and resid 408 and name CB)	15.68	1.30	1.31
	assign (segid 3A4 and resid 303 and name CA)	(segid 3A4 and resid 409 and name CA)	13.72	1.00	1.00
35	assign (segid 3A4 and resid 303 and name CA)	(segid 3A4 and resid 409 and name CB)	12.59	0.92	0.92
	assign (segid 3A4 and resid 303 and name CA)	(segid 3A4 and resid 410 and name CA)	13.86	1.11	1.11
	assign (segid 3A4 and resid 303 and name CA)	(segid 3A4 and resid 411 and name CA)	17.45	1.21	1.21
	assign (segid 3A4 and resid 303 and name CA)	(segid 3A4 and resid 304 and name C)	5.60	0.12	0.12
	assign (segid 3A4 and resid 303 and name CB)	(segid 3A4 and resid 304 and name CA)	4.57	0.10	0.11
40	assign (segid 3A4 and resid 303 and name CB)	(segid 3A4 and resid 304 and name CB)	5.40	0.12	0.11
	assign (segid 3A4 and resid 303 and name CB)	(segid 3A4 and resid 304 and name N)	3.28	0.12	0.12
	assign (segid 3A4 and resid 303 and name CB)	(segid 3A4 and resid 304 and name O)	6.62	0.22	0.22
	assign (segid 3A4 and resid 303 and name CB)	(segid 3A4 and resid 305 and name C)	7.42	0.28	0.27
	assign (segid 3A4 and resid 303 and name CB)	(segid 3A4 and resid 305 and name CA)	6.94	0.10	0.10
45	assign (segid 3A4 and resid 303 and name CB)	(segid 3A4 and resid 305 and name CB)	7.26	0.19	0.18
	assign (segid 3A4 and resid 303 and name CB)	(segid 3A4 and resid 305 and name N)	5.68	0.08	0.07
	assign (segid 3A4 and resid 303 and name CB)	(segid 3A4 and resid 306 and name CA)	7.59	0.63	0.64
	assign (segid 3A4 and resid 303 and name CB)	(segid 3A4 and resid 306 and name N)	6.78	0.44	0.43
	assign (segid 3A4 and resid 303 and name CB)	(segid 3A4 and resid 307 and name CA)	8.34	0.84	0.83
50	assign (segid 3A4 and resid 303 and name CB)	(segid 3A4 and resid 307 and name CB)	7.72	0.81	0.81
	assign (segid 3A4 and resid 303 and name CB)	(segid 3A4 and resid 308 and name CA)	10.32	0.37	0.36
	assign (segid 3A4 and resid 303 and name CB)	(segid 3A4 and resid 308 and name CB)	10.07	0.16	0.15
	assign (segid 3A4 and resid 303 and name CB)	(segid 3A4 and resid 309 and name CA)	12.13	0.43	0.44
	assign (segid 3A4 and resid 303 and name CB)	(segid 3A4 and resid 309 and name CB)	11.83	0.38	0.37
55	assign (segid 3A4 and resid 303 and name CB)	(segid 3A4 and resid 310 and name CA)	13.02	0.95	0.95
	assign (segid 3A4 and resid 303 and name CB)	(segid 3A4 and resid 310 and name CB)	12.31	1.12	1.12
	assign (segid 3A4 and resid 303 and name CB)	(segid 3A4 and resid 311 and name CA)	14.31	0.78	0.78
	assign (segid 3A4 and resid 303 and name CB)	(segid 3A4 and resid 311 and name CB)	13.69	0.71	0.70
	assign (segid 3A4 and resid 303 and name CB)	(segid 3A4 and resid 312 and name CA)	16.17	0.47	0.48
60	assign (segid 3A4 and resid 303 and name CB)	(segid 3A4 and resid 312 and name CB)	15.79	0.34	0.34
	assign (segid 3A4 and resid 303 and name CB)	(segid 3A4 and resid 313 and name CA)	17.81	0.72	0.73
	assign (segid 3A4 and resid 303 and name CB)	(segid 3A4 and resid 313 and name CB)	17.32	0.78	0.77
	assign (segid 3A4 and resid 303 and name CB)	(segid 3A4 and resid 314 and name CA)	18.75	0.95	0.95
	assign (segid 3A4 and resid 303 and name CB)	(segid 3A4 and resid 314 and name CB)	18.00	1.01	1.02
65	assign (segid 3A4 and resid 303 and name CB)	(segid 3A4 and resid 363 and name CA)	17.91	0.57	0.57
	assign (segid 3A4 and resid 303 and name CB)	(segid 3A4 and resid 363 and name CB)	18.01	0.51	0.51
	assign (segid 3A4 and resid 303 and name CB)	(segid 3A4 and resid 364 and name CA)	15.11	0.54	0.54
	assign (segid 3A4 and resid 303 and name CB)	(segid 3A4 and resid 364 and name CB)	15.80	0.58	0.58
	assign (segid 3A4 and resid 303 and name CB)	(segid 3A4 and resid 365 and name CA)	11.47	0.57	0.58
70	assign (segid 3A4 and resid 303 and name CB)	(segid 3A4 and resid 365 and name CB)	10.67	0.54	0.54
	assign (segid 3A4 and resid 303 and name CB)	(segid 3A4 and resid 395 and name CA)	18.04	0.99	0.98
	assign (segid 3A4 and resid 303 and name CB)	(segid 3A4 and resid 398 and name CA)	14.99	0.83	0.82
	assign (segid 3A4 and resid 303 and name CB)	(segid 3A4 and resid 398 and name CB)	14.46	0.86	0.86
	assign (segid 3A4 and resid 303 and name CB)	(segid 3A4 and resid 399 and name CA)	14.77	0.89	0.90
75	assign (segid 3A4 and resid 303 and name CB)	(segid 3A4 and resid 399 and name CB)	15.70	0.92	0.91
	assign (segid 3A4 and resid 303 and name CB)	(segid 3A4 and resid 400 and name CA)	16.91	0.90	0.90
	assign (segid 3A4 and resid 303 and name CB)	(segid 3A4 and resid 400 and name CB)	18.28	0.87	0.88
	assign (segid 3A4 and resid 303 and name CB)	(segid 3A4 and resid 401 and name CA)	15.12	0.65	0.65
	assign (segid 3A4 and resid 303 and name CB)	(segid 3A4 and resid 402 and name CA)	11.71	0.77	0.77
80	assign (segid 3A4 and resid 303 and name CB)	(segid 3A4 and resid 402 and name CB)	10.96	0.77	0.76
	assign (segid 3A4 and resid 303 and name CB)	(segid 3A4 and resid 403 and name CA)	13.63	1.05	1.06
	assign (segid 3A4 and resid 303 and name CB)	(segid 3A4 and resid 403 and name CB)	14.74	1.02	1.02

	assign (segid 3A4 and resid 303 and name CB)	(segid 3A4 and resid 404 and name CA)	15.84	1.15	1.15
	assign (segid 3A4 and resid 303 and name CB)	(segid 3A4 and resid 404 and name CB)	16.78	1.09	1.08
	assign (segid 3A4 and resid 303 and name CB)	(segid 3A4 and resid 405 and name CA)	13.57	1.23	1.23
	assign (segid 3A4 and resid 303 and name CB)	(segid 3A4 and resid 405 and name CB)	12.90	1.01	1.00
5	assign (segid 3A4 and resid 303 and name CB)	(segid 3A4 and resid 406 and name CA)	11.46	1.39	1.39
	assign (segid 3A4 and resid 303 and name CB)	(segid 3A4 and resid 407 and name CA)	14.91	1.45	1.44
	assign (segid 3A4 and resid 303 and name CB)	(segid 3A4 and resid 407 and name CB)	15.85	1.44	1.45
	assign (segid 3A4 and resid 303 and name CB)	(segid 3A4 and resid 408 and name CA)	16.78	1.31	1.31
	assign (segid 3A4 and resid 303 and name CB)	(segid 3A4 and resid 408 and name CB)	17.08	1.31	1.31
	assign (segid 3A4 and resid 303 and name CB)	(segid 3A4 and resid 409 and name CA)	14.94	1.02	1.02
10	assign (segid 3A4 and resid 303 and name CB)	(segid 3A4 and resid 409 and name CB)	13.81	0.95	0.94
	assign (segid 3A4 and resid 303 and name CB)	(segid 3A4 and resid 410 and name CA)	14.91	1.16	1.15
	assign (segid 3A4 and resid 303 and name CB)	(segid 3A4 and resid 303 and name C)	2.47	0.02	0.03
	assign (segid 3A4 and resid 303 and name N)	(segid 3A4 and resid 303 and name CA)	1.46	0.00	0.00
	assign (segid 3A4 and resid 303 and name N)	(segid 3A4 and resid 303 and name CB)	2.44	0.05	0.04
15	assign (segid 3A4 and resid 303 and name N)	(segid 3A4 and resid 303 and name O)	3.58	0.05	0.04
	assign (segid 3A4 and resid 303 and name N)	(segid 3A4 and resid 304 and name C)	4.79	0.04	0.04
	assign (segid 3A4 and resid 303 and name N)	(segid 3A4 and resid 304 and name CA)	4.17	0.10	0.09
	assign (segid 3A4 and resid 303 and name N)	(segid 3A4 and resid 304 and name CB)	4.90	0.16	0.16
	assign (segid 3A4 and resid 303 and name N)	(segid 3A4 and resid 304 and name N)	2.75	0.11	0.11
20	assign (segid 3A4 and resid 303 and name N)	(segid 3A4 and resid 304 and name O)	5.96	0.07	0.06
	assign (segid 3A4 and resid 303 and name N)	(segid 3A4 and resid 305 and name C)	6.34	0.35	0.35
	assign (segid 3A4 and resid 303 and name N)	(segid 3A4 and resid 305 and name CA)	5.55	0.10	0.11
	assign (segid 3A4 and resid 303 and name N)	(segid 3A4 and resid 305 and name CB)	5.55	0.17	0.16
	assign (segid 3A4 and resid 303 and name N)	(segid 3A4 and resid 305 and name N)	4.42	0.08	0.09
25	assign (segid 3A4 and resid 303 and name N)	(segid 3A4 and resid 305 and name O)	7.50	0.33	0.34
	assign (segid 3A4 and resid 303 and name N)	(segid 3A4 and resid 306 and name N)	5.97	0.64	0.63
	assign (segid 3A4 and resid 303 and name N)	(segid 3A4 and resid 303 and name CB)	3.13	0.12	0.12
	assign (segid 3A4 and resid 303 and name O)	(segid 3A4 and resid 304 and name C)	3.31	0.19	0.19
	assign (segid 3A4 and resid 303 and name O)	(segid 3A4 and resid 304 and name CA)	2.79	0.04	0.05
30	assign (segid 3A4 and resid 303 and name O)	(segid 3A4 and resid 304 and name CB)	4.22	0.03	0.02
	assign (segid 3A4 and resid 303 and name O)	(segid 3A4 and resid 304 and name N)	2.25	0.01	0.02
	assign (segid 3A4 and resid 303 and name O)	(segid 3A4 and resid 304 and name O)	4.04	0.37	0.37
	assign (segid 3A4 and resid 303 and name O)	(segid 3A4 and resid 305 and name C)	4.77	0.36	0.35
	assign (segid 3A4 and resid 303 and name O)	(segid 3A4 and resid 305 and name CA)	4.71	0.16	0.17
35	assign (segid 3A4 and resid 303 and name O)	(segid 3A4 and resid 305 and name CB)	5.46	0.17	0.17
	assign (segid 3A4 and resid 303 and name O)	(segid 3A4 and resid 305 and name N)	3.61	0.12	0.12
	assign (segid 3A4 and resid 303 and name O)	(segid 3A4 and resid 305 and name O)	5.80	0.47	0.47
	assign (segid 3A4 and resid 303 and name O)	(segid 3A4 and resid 306 and name C)	5.13	0.82	0.82
	assign (segid 3A4 and resid 303 and name O)	(segid 3A4 and resid 306 and name CA)	4.76	0.62	0.62
40	assign (segid 3A4 and resid 303 and name O)	(segid 3A4 and resid 306 and name N)	4.05	0.43	0.44
	assign (segid 3A4 and resid 303 and name O)	(segid 3A4 and resid 306 and name O)	6.33	0.85	0.85
	assign (segid 3A4 and resid 303 and name O)	(segid 3A4 and resid 307 and name C)	6.40	0.82	0.83
	assign (segid 3A4 and resid 303 and name O)	(segid 3A4 and resid 307 and name CA)	5.34	0.91	0.92
	assign (segid 3A4 and resid 303 and name O)	(segid 3A4 and resid 307 and name CB)	4.95	0.83	0.83
45	assign (segid 3A4 and resid 303 and name O)	(segid 3A4 and resid 307 and name N)	4.44	0.89	0.90
	assign (segid 3A4 and resid 303 and name O)	(segid 3A4 and resid 308 and name CB)	7.46	0.40	0.40
	assign (segid 3A4 and resid 303 and name O)	(segid 3A4 and resid 308 and name N)	6.25	0.68	0.68
	assign (segid 3A4 and resid 303 and name O)	(segid 3A4 and resid 308 and name CB)	2.49	0.01	0.01
	assign (segid 3A4 and resid 304 and name C)	(segid 3A4 and resid 304 and name O)	1.24	0.02	0.01
50	assign (segid 3A4 and resid 304 and name C)	(segid 3A4 and resid 305 and name C)	3.01	0.07	0.07
	assign (segid 3A4 and resid 304 and name C)	(segid 3A4 and resid 305 and name CA)	2.44	0.01	0.01
	assign (segid 3A4 and resid 304 and name C)	(segid 3A4 and resid 305 and name CB)	3.74	0.03	0.02
	assign (segid 3A4 and resid 304 and name C)	(segid 3A4 and resid 305 and name N)	1.33	0.01	0.01
	assign (segid 3A4 and resid 304 and name C)	(segid 3A4 and resid 305 and name O)	3.82	0.08	0.07
55	assign (segid 3A4 and resid 304 and name C)	(segid 3A4 and resid 306 and name C)	4.63	0.15	0.15
	assign (segid 3A4 and resid 304 and name C)	(segid 3A4 and resid 306 and name CA)	4.51	0.14	0.13
	assign (segid 3A4 and resid 304 and name C)	(segid 3A4 and resid 306 and name N)	3.31	0.12	0.13
	assign (segid 3A4 and resid 304 and name C)	(segid 3A4 and resid 306 and name O)	5.73	0.15	0.14
60	assign (segid 3A4 and resid 304 and name C)	(segid 3A4 and resid 307 and name C)	4.88	0.09	0.09
	assign (segid 3A4 and resid 304 and name C)	(segid 3A4 and resid 307 and name CA)	4.57	0.17	0.17
	assign (segid 3A4 and resid 304 and name C)	(segid 3A4 and resid 307 and name CB)	4.31	0.24	0.25
	assign (segid 3A4 and resid 304 and name C)	(segid 3A4 and resid 307 and name N)	3.88	0.18	0.17
	assign (segid 3A4 and resid 304 and name C)	(segid 3A4 and resid 307 and name O)	6.07	0.07	0.07
	assign (segid 3A4 and resid 304 and name C)	(segid 3A4 and resid 308 and name C)	6.15	0.09	0.08
65	assign (segid 3A4 and resid 304 and name C)	(segid 3A4 and resid 308 and name CA)	5.02	0.09	0.08
	assign (segid 3A4 and resid 304 and name C)	(segid 3A4 and resid 308 and name CB)	4.57	0.16	0.16
	assign (segid 3A4 and resid 304 and name C)	(segid 3A4 and resid 308 and name N)	4.14	0.06	0.06
	assign (segid 3A4 and resid 304 and name C)	(segid 3A4 and resid 308 and name O)	7.29	0.09	0.09
70	assign (segid 3A4 and resid 304 and name C)	(segid 3A4 and resid 309 and name CA)	7.39	0.12	0.12
	assign (segid 3A4 and resid 304 and name C)	(segid 3A4 and resid 309 and name CB)	7.49	0.17	0.17
	assign (segid 3A4 and resid 304 and name C)	(segid 3A4 and resid 309 and name N)	6.08	0.11	0.10
	assign (segid 3A4 and resid 304 and name C)	(segid 3A4 and resid 309 and name O)	7.17	0.31	0.32
	assign (segid 3A4 and resid 304 and name C)	(segid 3A4 and resid 365 and name C)	7.19	0.20	0.19
	assign (segid 3A4 and resid 304 and name C)	(segid 3A4 and resid 365 and name CB)	6.12	0.14	0.15
75	assign (segid 3A4 and resid 304 and name C)	(segid 3A4 and resid 365 and name O)	6.59	0.48	0.49
	assign (segid 3A4 and resid 304 and name C)	(segid 3A4 and resid 304 and name O)	1.52	0.00	0.01
	assign (segid 3A4 and resid 304 and name CA)	(segid 3A4 and resid 304 and name CB)	1.53	0.00	0.01
	assign (segid 3A4 and resid 304 and name CA)	(segid 3A4 and resid 304 and name O)	2.38	0.02	0.02
80	assign (segid 3A4 and resid 304 and name CA)	(segid 3A4 and resid 305 and name C)	4.43	0.07	0.06
	assign (segid 3A4 and resid 304 and name CA)	(segid 3A4 and resid 305 and name CA)	3.83	0.02	0.03
	assign (segid 3A4 and resid 304 and name CA)	(segid 3A4 and resid 305 and name CB)	4.92	0.05	0.06
	assign (segid 3A4 and resid 304 and name CA)	(segid 3A4 and resid 305 and name N)	2.47	0.04	0.03

	assign (segid 3A4 and resid 304 and name CA) (segid 3A4 and resid 305 and name O)	5.29	0.08	0.08
	assign (segid 3A4 and resid 304 and name CA) (segid 3A4 and resid 306 and name C)	5.62	0.21	0.21
	assign (segid 3A4 and resid 304 and name CA) (segid 3A4 and resid 306 and name CA)	5.54	0.17	0.17
	assign (segid 3A4 and resid 304 and name CA) (segid 3A4 and resid 306 and name N)	4.45	0.13	0.14
5	assign (segid 3A4 and resid 304 and name CA) (segid 3A4 and resid 306 and name O)	6.76	0.21	0.21
	assign (segid 3A4 and resid 304 and name CA) (segid 3A4 and resid 307 and name C)	5.75	0.17	0.16
	assign (segid 3A4 and resid 304 and name CA) (segid 3A4 and resid 307 and name CA)	5.21	0.27	0.26
	assign (segid 3A4 and resid 304 and name CA) (segid 3A4 and resid 307 and name CB)	4.54	0.34	0.34
	assign (segid 3A4 and resid 304 and name CA) (segid 3A4 and resid 307 and name N)	4.68	0.25	0.24
10	assign (segid 3A4 and resid 304 and name CA) (segid 3A4 and resid 307 and name O)	6.90	0.14	0.14
	assign (segid 3A4 and resid 304 and name CA) (segid 3A4 and resid 308 and name C)	7.42	0.10	0.10
	assign (segid 3A4 and resid 304 and name CA) (segid 3A4 and resid 308 and name CA)	6.18	0.09	0.10
	assign (segid 3A4 and resid 304 and name CA) (segid 3A4 and resid 308 and name CB)	5.83	0.17	0.18
	assign (segid 3A4 and resid 304 and name CA) (segid 3A4 and resid 308 and name N)	5.22	0.11	0.11
	assign (segid 3A4 and resid 304 and name CA) (segid 3A4 and resid 309 and name CA)	8.77	0.11	0.12
15	assign (segid 3A4 and resid 304 and name CA) (segid 3A4 and resid 309 and name CB)	8.90	0.16	0.15
	assign (segid 3A4 and resid 304 and name CA) (segid 3A4 and resid 309 and name N)	7.44	0.11	0.11
	assign (segid 3A4 and resid 304 and name CA) (segid 3A4 and resid 310 and name CA)	9.99	0.22	0.23
	assign (segid 3A4 and resid 304 and name CA) (segid 3A4 and resid 310 and name CB)	9.57	0.31	0.32
20	assign (segid 3A4 and resid 304 and name CA) (segid 3A4 and resid 311 and name CA)	10.56	0.19	0.18
	assign (segid 3A4 and resid 304 and name CA) (segid 3A4 and resid 311 and name CB)	9.75	0.20	0.20
	assign (segid 3A4 and resid 304 and name CA) (segid 3A4 and resid 312 and name CA)	12.25	0.09	0.09
	assign (segid 3A4 and resid 304 and name CA) (segid 3A4 and resid 312 and name CB)	11.90	0.14	0.14
	assign (segid 3A4 and resid 304 and name CA) (segid 3A4 and resid 313 and name CA)	14.43	0.16	0.16
25	assign (segid 3A4 and resid 304 and name CA) (segid 3A4 and resid 313 and name CB)	14.20	0.22	0.22
	assign (segid 3A4 and resid 304 and name CA) (segid 3A4 and resid 314 and name CA)	15.31	0.20	0.19
	assign (segid 3A4 and resid 304 and name CA) (segid 3A4 and resid 314 and name CB)	14.59	0.22	0.23
	assign (segid 3A4 and resid 304 and name CA) (segid 3A4 and resid 315 and name CA)	16.23	0.23	0.23
	assign (segid 3A4 and resid 304 and name CA) (segid 3A4 and resid 315 and name CB)	15.39	0.30	0.31
30	assign (segid 3A4 and resid 304 and name CA) (segid 3A4 and resid 316 and name CA)	18.05	0.23	0.23
	assign (segid 3A4 and resid 304 and name CA) (segid 3A4 and resid 317 and name CA)	18.64	0.85	0.85
	assign (segid 3A4 and resid 304 and name CA) (segid 3A4 and resid 317 and name CB)	18.02	0.79	0.78
	assign (segid 3A4 and resid 304 and name CA) (segid 3A4 and resid 319 and name CB)	19.09	0.30	0.31
	assign (segid 3A4 and resid 304 and name CA) (segid 3A4 and resid 320 and name CA)	19.07	0.37	0.38
35	assign (segid 3A4 and resid 304 and name CA) (segid 3A4 and resid 321 and name CA)	16.92	0.21	0.21
	assign (segid 3A4 and resid 304 and name CA) (segid 3A4 and resid 322 and name CB)	16.92	0.26	0.27
	assign (segid 3A4 and resid 304 and name CA) (segid 3A4 and resid 323 and name CA)	13.67	0.24	0.24
	assign (segid 3A4 and resid 304 and name CA) (segid 3A4 and resid 324 and name CB)	13.67	0.29	0.29
	assign (segid 3A4 and resid 304 and name CA) (segid 3A4 and resid 325 and name CA)	11.11	0.18	0.19
40	assign (segid 3A4 and resid 304 and name CA) (segid 3A4 and resid 326 and name CB)	12.00	0.22	0.22
	assign (segid 3A4 and resid 304 and name CA) (segid 3A4 and resid 327 and name C)	7.19	0.27	0.26
	assign (segid 3A4 and resid 304 and name CA) (segid 3A4 and resid 328 and name CA)	7.46	0.19	0.18
	assign (segid 3A4 and resid 304 and name CA) (segid 3A4 and resid 329 and name CB)	6.46	0.19	0.18
	assign (segid 3A4 and resid 304 and name CA) (segid 3A4 and resid 330 and name O)	6.59	0.41	0.41
45	assign (segid 3A4 and resid 304 and name CA) (segid 3A4 and resid 331 and name CA)	17.47	0.51	0.51
	assign (segid 3A4 and resid 304 and name CA) (segid 3A4 and resid 332 and name CA)	19.04	0.28	0.27
	assign (segid 3A4 and resid 304 and name CA) (segid 3A4 and resid 333 and name CA)	17.50	0.85	0.85
	assign (segid 3A4 and resid 304 and name CA) (segid 3A4 and resid 334 and name CB)	17.10	0.67	0.67
50	assign (segid 3A4 and resid 304 and name CA) (segid 3A4 and resid 335 and name CB)	17.50	0.67	0.67
	assign (segid 3A4 and resid 304 and name CA) (segid 3A4 and resid 336 and name CA)	13.54	0.71	0.71
	assign (segid 3A4 and resid 304 and name CA) (segid 3A4 and resid 337 and name CB)	13.20	0.75	0.76
	assign (segid 3A4 and resid 304 and name CA) (segid 3A4 and resid 338 and name CA)	14.08	0.72	0.73
	assign (segid 3A4 and resid 304 and name CA) (segid 3A4 and resid 339 and name CB)	15.31	0.74	0.74
	assign (segid 3A4 and resid 304 and name CA) (segid 3A4 and resid 340 and name CA)	15.58	0.72	0.72
55	assign (segid 3A4 and resid 304 and name CA) (segid 3A4 and resid 341 and name CB)	16.82	0.67	0.68
	assign (segid 3A4 and resid 304 and name CA) (segid 3A4 and resid 342 and name CA)	12.97	0.58	0.57
	assign (segid 3A4 and resid 304 and name CA) (segid 3A4 and resid 343 and name CB)	10.11	0.71	0.70
	assign (segid 3A4 and resid 304 and name CA) (segid 3A4 and resid 344 and name CB)	9.77	0.68	0.67
	assign (segid 3A4 and resid 304 and name CA) (segid 3A4 and resid 345 and name CA)	12.74	0.82	0.82
60	assign (segid 3A4 and resid 304 and name CA) (segid 3A4 and resid 346 and name CB)	14.07	0.79	0.80
	assign (segid 3A4 and resid 304 and name CA) (segid 3A4 and resid 347 and name CA)	14.05	0.98	0.98
	assign (segid 3A4 and resid 304 and name CA) (segid 3A4 and resid 348 and name CB)	14.73	0.98	0.99
	assign (segid 3A4 and resid 304 and name CA) (segid 3A4 and resid 349 and name CA)	11.13	1.10	1.10
	assign (segid 3A4 and resid 304 and name CA) (segid 3A4 and resid 350 and name CB)	10.14	0.99	1.00
65	assign (segid 3A4 and resid 304 and name CA) (segid 3A4 and resid 351 and name CA)	10.08	0.99	0.98
	assign (segid 3A4 and resid 304 and name CA) (segid 3A4 and resid 352 and name CB)	13.79	0.97	0.97
	assign (segid 3A4 and resid 304 and name CA) (segid 3A4 and resid 353 and name CB)	14.85	0.98	0.99
	assign (segid 3A4 and resid 304 and name CA) (segid 3A4 and resid 354 and name CA)	14.76	0.93	0.93
	assign (segid 3A4 and resid 304 and name CA) (segid 3A4 and resid 355 and name CB)	14.73	1.01	1.00
70	assign (segid 3A4 and resid 304 and name CA) (segid 3A4 and resid 356 and name CA)	12.75	0.69	0.69
	assign (segid 3A4 and resid 304 and name CA) (segid 3A4 and resid 357 and name CB)	11.41	0.72	0.73
	assign (segid 3A4 and resid 304 and name CA) (segid 3A4 and resid 358 and name CA)	13.77	0.54	0.54
	assign (segid 3A4 and resid 304 and name CA) (segid 3A4 and resid 359 and name CB)	17.23	0.64	0.65
	assign (segid 3A4 and resid 304 and name CA) (segid 3A4 and resid 360 and name CA)	17.83	0.80	0.81
75	assign (segid 3A4 and resid 304 and name CA) (segid 3A4 and resid 361 and name CB)	17.65	0.65	0.66
	assign (segid 3A4 and resid 304 and name CB) (segid 3A4 and resid 305 and name C)	5.46	0.09	0.09
	assign (segid 3A4 and resid 304 and name CB) (segid 3A4 and resid 305 and name CA)	4.65	0.09	0.09
	assign (segid 3A4 and resid 304 and name CB) (segid 3A4 and resid 305 and name CB)	5.71	0.14	0.14
	assign (segid 3A4 and resid 304 and name CB) (segid 3A4 and resid 305 and name N)	3.38	0.11	0.11
80	assign (segid 3A4 and resid 304 and name CB) (segid 3A4 and resid 305 and name O)	6.17	0.10	0.11
	assign (segid 3A4 and resid 304 and name CB) (segid 3A4 and resid 306 and name C)	6.80	0.16	0.15
	assign (segid 3A4 and resid 304 and name CB) (segid 3A4 and resid 306 and name CA)	6.84	0.14	0.15
	assign (segid 3A4 and resid 304 and name CB) (segid 3A4 and resid 306 and name N)	5.72	0.14	0.14

	assign (segid 3A4 and resid 304 and name N)	(segid 3A4 and resid 307 and name CB)	5.61	0.50	0.49
	assign (segid 3A4 and resid 304 and name N)	(segid 3A4 and resid 307 and name N)	5.44	0.46	0.47
	assign (segid 3A4 and resid 304 and name N)	(segid 3A4 and resid 308 and name CA)	7.38	0.11	0.10
	assign (segid 3A4 and resid 304 and name N)	(segid 3A4 and resid 308 and name CB)	6.96	0.17	0.17
	assign (segid 3A4 and resid 304 and name N)	(segid 3A4 and resid 308 and name N)	6.38	0.19	0.20
5	assign (segid 3A4 and resid 304 and name O)	(segid 3A4 and resid 304 and name CB)	3.06	0.13	0.13
	assign (segid 3A4 and resid 304 and name O)	(segid 3A4 and resid 305 and name C)	2.89	0.12	0.12
	assign (segid 3A4 and resid 304 and name O)	(segid 3A4 and resid 305 and name CA)	2.75	0.02	0.02
	assign (segid 3A4 and resid 304 and name O)	(segid 3A4 and resid 305 and name CB)	4.26	0.02	0.01
	assign (segid 3A4 and resid 304 and name O)	(segid 3A4 and resid 305 and name N)	2.25	0.01	0.00
10	assign (segid 3A4 and resid 304 and name O)	(segid 3A4 and resid 305 and name O)	3.33	0.13	0.13
	assign (segid 3A4 and resid 304 and name O)	(segid 3A4 and resid 306 and name C)	4.06	0.23	0.23
	assign (segid 3A4 and resid 304 and name O)	(segid 3A4 and resid 306 and name CA)	4.30	0.21	0.22
	assign (segid 3A4 and resid 304 and name O)	(segid 3A4 and resid 306 and name N)	3.36	0.19	0.19
	assign (segid 3A4 and resid 304 and name O)	(segid 3A4 and resid 306 and name O)	5.02	0.21	0.22
15	assign (segid 3A4 and resid 304 and name O)	(segid 3A4 and resid 307 and name C)	3.75	0.13	0.12
	assign (segid 3A4 and resid 304 and name O)	(segid 3A4 and resid 307 and name CA)	3.66	0.23	0.23
	assign (segid 3A4 and resid 304 and name O)	(segid 3A4 and resid 307 and name CB)	3.51	0.29	0.28
	assign (segid 3A4 and resid 304 and name O)	(segid 3A4 and resid 307 and name N)	3.21	0.24	0.25
	assign (segid 3A4 and resid 304 and name O)	(segid 3A4 and resid 307 and name O)	4.91	0.08	0.08
20	assign (segid 3A4 and resid 304 and name O)	(segid 3A4 and resid 308 and name C)	5.07	0.11	0.10
	assign (segid 3A4 and resid 304 and name O)	(segid 3A4 and resid 308 and name CA)	3.86	0.10	0.10
	assign (segid 3A4 and resid 304 and name O)	(segid 3A4 and resid 308 and name CB)	3.61	0.17	0.16
	assign (segid 3A4 and resid 304 and name O)	(segid 3A4 and resid 308 and name N)	2.97	0.10	0.10
	assign (segid 3A4 and resid 304 and name O)	(segid 3A4 and resid 308 and name O)	6.17	0.10	0.11
25	assign (segid 3A4 and resid 304 and name O)	(segid 3A4 and resid 309 and name C)	7.29	0.14	0.14
	assign (segid 3A4 and resid 304 and name O)	(segid 3A4 and resid 309 and name CA)	6.51	0.15	0.15
	assign (segid 3A4 and resid 304 and name O)	(segid 3A4 and resid 309 and name CB)	6.81	0.21	0.20
	assign (segid 3A4 and resid 304 and name O)	(segid 3A4 and resid 309 and name N)	5.13	0.14	0.14
	assign (segid 3A4 and resid 304 and name O)	(segid 3A4 and resid 310 and name N)	6.91	0.17	0.16
30	assign (segid 3A4 and resid 304 and name O)	(segid 3A4 and resid 311 and name N)	7.68	0.14	0.13
	assign (segid 3A4 and resid 304 and name O)	(segid 3A4 and resid 311 and name C)	6.21	0.34	0.35
	assign (segid 3A4 and resid 304 and name O)	(segid 3A4 and resid 365 and name N)	6.13	0.22	0.21
	assign (segid 3A4 and resid 304 and name O)	(segid 3A4 and resid 365 and name CA)	5.13	0.17	0.16
	assign (segid 3A4 and resid 304 and name O)	(segid 3A4 and resid 365 and name CB)	7.42	0.20	0.20
35	assign (segid 3A4 and resid 304 and name O)	(segid 3A4 and resid 365 and name N)	5.65	0.52	0.51
	assign (segid 3A4 and resid 304 and name O)	(segid 3A4 and resid 365 and name CB)	2.53	0.03	0.04
	assign (segid 3A4 and resid 305 and name C)	(segid 3A4 and resid 305 and name O)	1.23	0.00	0.01
	assign (segid 3A4 and resid 305 and name C)	(segid 3A4 and resid 306 and name C)	3.04	0.05	0.04
	assign (segid 3A4 and resid 305 and name C)	(segid 3A4 and resid 306 and name CA)	2.45	0.01	0.01
40	assign (segid 3A4 and resid 305 and name C)	(segid 3A4 and resid 306 and name N)	1.33	0.01	0.02
	assign (segid 3A4 and resid 305 and name C)	(segid 3A4 and resid 306 and name O)	3.91	0.08	0.07
	assign (segid 3A4 and resid 305 and name C)	(segid 3A4 and resid 307 and name C)	4.46	0.04	0.04
	assign (segid 3A4 and resid 305 and name C)	(segid 3A4 and resid 307 and name CA)	4.40	0.07	0.08
	assign (segid 3A4 and resid 305 and name C)	(segid 3A4 and resid 307 and name CB)	5.11	0.10	0.11
45	assign (segid 3A4 and resid 305 and name C)	(segid 3A4 and resid 307 and name N)	3.25	0.09	0.09
	assign (segid 3A4 and resid 305 and name C)	(segid 3A4 and resid 307 and name O)	5.57	0.03	0.03
	assign (segid 3A4 and resid 305 and name C)	(segid 3A4 and resid 308 and name C)	4.77	0.05	0.05
	assign (segid 3A4 and resid 305 and name C)	(segid 3A4 and resid 308 and name CA)	4.36	0.04	0.05
	assign (segid 3A4 and resid 305 and name C)	(segid 3A4 and resid 308 and name CB)	4.06	0.09	0.08
50	assign (segid 3A4 and resid 305 and name C)	(segid 3A4 and resid 308 and name N)	3.66	0.06	0.07
	assign (segid 3A4 and resid 305 and name C)	(segid 3A4 and resid 308 and name O)	5.98	0.05	0.06
	assign (segid 3A4 and resid 305 and name C)	(segid 3A4 and resid 309 and name C)	6.16	0.06	0.06
	assign (segid 3A4 and resid 305 and name C)	(segid 3A4 and resid 309 and name CA)	5.08	0.10	0.11
	assign (segid 3A4 and resid 305 and name C)	(segid 3A4 and resid 309 and name CB)	4.79	0.17	0.17
55	assign (segid 3A4 and resid 305 and name C)	(segid 3A4 and resid 309 and name N)	4.10	0.07	0.07
	assign (segid 3A4 and resid 305 and name C)	(segid 3A4 and resid 309 and name O)	7.32	0.07	0.07
	assign (segid 3A4 and resid 305 and name C)	(segid 3A4 and resid 310 and name CA)	7.32	0.11	0.11
	assign (segid 3A4 and resid 305 and name C)	(segid 3A4 and resid 310 and name CB)	7.36	0.18	0.18
	assign (segid 3A4 and resid 305 and name C)	(segid 3A4 and resid 310 and name N)	6.02	0.08	0.09
60	assign (segid 3A4 and resid 305 and name C)	(segid 3A4 and resid 311 and name N)	7.77	0.08	0.07
	assign (segid 3A4 and resid 305 and name C)	(segid 3A4 and resid 365 and name CB)	7.33	0.08	0.09
	assign (segid 3A4 and resid 305 and name C)	(segid 3A4 and resid 402 and name CA)	6.06	0.65	0.64
	assign (segid 3A4 and resid 305 and name C)	(segid 3A4 and resid 402 and name CB)	5.85	0.61	0.61
	assign (segid 3A4 and resid 305 and name C)	(segid 3A4 and resid 402 and name O)	6.70	0.65	0.65
65	assign (segid 3A4 and resid 305 and name CA)	(segid 3A4 and resid 305 and name C)	1.53	0.01	0.02
	assign (segid 3A4 and resid 305 and name CA)	(segid 3A4 and resid 305 and name CB)	1.54	0.01	0.01
	assign (segid 3A4 and resid 305 and name CA)	(segid 3A4 and resid 305 and name O)	2.40	0.02	0.02
	assign (segid 3A4 and resid 305 and name CA)	(segid 3A4 and resid 306 and name C)	4.46	0.03	0.04
	assign (segid 3A4 and resid 305 and name CA)	(segid 3A4 and resid 306 and name CA)	3.85	0.02	0.02
70	assign (segid 3A4 and resid 305 and name CA)	(segid 3A4 and resid 306 and name N)	2.47	0.03	0.03
	assign (segid 3A4 and resid 305 and name CA)	(segid 3A4 and resid 306 and name O)	5.39	0.07	0.08
	assign (segid 3A4 and resid 305 and name CA)	(segid 3A4 and resid 307 and name C)	5.43	0.05	0.05
	assign (segid 3A4 and resid 305 and name CA)	(segid 3A4 and resid 307 and name CA)	5.43	0.07	0.07
	assign (segid 3A4 and resid 305 and name CA)	(segid 3A4 and resid 307 and name CB)	5.80	0.12	0.13
75	assign (segid 3A4 and resid 305 and name CA)	(segid 3A4 and resid 307 and name N)	4.39	0.08	0.09
	assign (segid 3A4 and resid 305 and name CA)	(segid 3A4 and resid 307 and name O)	6.56	0.05	0.05
	assign (segid 3A4 and resid 305 and name CA)	(segid 3A4 and resid 308 and name C)	5.62	0.08	0.08
	assign (segid 3A4 and resid 305 and name CA)	(segid 3A4 and resid 308 and name CA)	4.95	0.08	0.08
80	assign (segid 3A4 and resid 305 and name CA)	(segid 3A4 and resid 308 and name CB)	4.20	0.13	0.14
	assign (segid 3A4 and resid 305 and name CA)	(segid 3A4 and resid 308 and name N)	4.43	0.07	0.07
	assign (segid 3A4 and resid 305 and name CA)	(segid 3A4 and resid 308 and name O)	6.80	0.10	0.10
	assign (segid 3A4 and resid 305 and name CA)	(segid 3A4 and resid 309 and name C)	7.42	0.06	0.06

	assign (segid 3A4 and resid 305 and name CA)	(segid 3A4 and resid 309 and name CA)	6.24	0.12	0.12
	assign (segid 3A4 and resid 305 and name CA)	(segid 3A4 and resid 309 and name CB)	6.05	0.18	0.17
	assign (segid 3A4 and resid 305 and name CA)	(segid 3A4 and resid 309 and name N)	5.17	0.07	0.08
	assign (segid 3A4 and resid 305 and name CA)	(segid 3A4 and resid 310 and name CA)	8.69	0.10	0.10
	assign (segid 3A4 and resid 305 and name CA)	(segid 3A4 and resid 310 and name CB)	8.76	0.18	0.17
5	assign (segid 3A4 and resid 305 and name CA)	(segid 3A4 and resid 310 and name N)	7.38	0.08	0.08
	assign (segid 3A4 and resid 305 and name CA)	(segid 3A4 and resid 311 and name CA)	9.80	0.12	0.12
	assign (segid 3A4 and resid 305 and name CA)	(segid 3A4 and resid 311 and name CB)	9.37	0.15	0.15
	assign (segid 3A4 and resid 305 and name CA)	(segid 3A4 and resid 312 and name CA)	10.40	0.15	0.15
	assign (segid 3A4 and resid 305 and name CA)	(segid 3A4 and resid 312 and name CB)	9.67	0.22	0.21
10	assign (segid 3A4 and resid 305 and name CA)	(segid 3A4 and resid 313 and name CA)	12.45	0.19	0.18
	assign (segid 3A4 and resid 305 and name CA)	(segid 3A4 and resid 313 and name CB)	12.16	0.23	0.23
	assign (segid 3A4 and resid 305 and name CA)	(segid 3A4 and resid 314 and name CA)	14.21	0.06	0.06
	assign (segid 3A4 and resid 305 and name CA)	(segid 3A4 and resid 314 and name CB)	13.85	0.07	0.08
	assign (segid 3A4 and resid 305 and name CA)	(segid 3A4 and resid 315 and name CA)	15.11	0.22	0.22
15	assign (segid 3A4 and resid 305 and name CA)	(segid 3A4 and resid 315 and name CB)	14.34	0.30	0.30
	assign (segid 3A4 and resid 305 and name CA)	(segid 3A4 and resid 316 and name CA)	16.18	0.30	0.31
	assign (segid 3A4 and resid 305 and name CA)	(segid 3A4 and resid 317 and name CA)	17.61	0.50	0.50
	assign (segid 3A4 and resid 305 and name CA)	(segid 3A4 and resid 318 and name CB)	18.22	0.68	0.69
	assign (segid 3A4 and resid 305 and name CA)	(segid 3A4 and resid 351 and name CA)	19.32	0.22	0.23
20	assign (segid 3A4 and resid 305 and name CA)	(segid 3A4 and resid 357 and name CB)	18.64	0.62	0.63
	assign (segid 3A4 and resid 305 and name CA)	(segid 3A4 and resid 360 and name CA)	19.44	0.20	0.19
	assign (segid 3A4 and resid 305 and name CA)	(segid 3A4 and resid 362 and name CA)	17.27	0.17	0.18
	assign (segid 3A4 and resid 305 and name CA)	(segid 3A4 and resid 362 and name CB)	17.61	0.21	0.20
	assign (segid 3A4 and resid 305 and name CA)	(segid 3A4 and resid 363 and name CA)	13.67	0.21	0.21
25	assign (segid 3A4 and resid 305 and name CA)	(segid 3A4 and resid 363 and name CB)	13.34	0.28	0.29
	assign (segid 3A4 and resid 305 and name CA)	(segid 3A4 and resid 364 and name CA)	12.04	0.17	0.18
	assign (segid 3A4 and resid 305 and name CA)	(segid 3A4 and resid 364 and name CB)	13.24	0.21	0.21
	assign (segid 3A4 and resid 305 and name CA)	(segid 3A4 and resid 365 and name CA)	8.48	0.23	0.23
	assign (segid 3A4 and resid 305 and name CA)	(segid 3A4 and resid 365 and name CB)	7.36	0.15	0.16
30	assign (segid 3A4 and resid 305 and name CA)	(segid 3A4 and resid 381 and name CA)	16.93	0.42	0.42
	assign (segid 3A4 and resid 305 and name CA)	(segid 3A4 and resid 382 and name CA)	19.07	0.16	0.16
	assign (segid 3A4 and resid 305 and name CA)	(segid 3A4 and resid 383 and name CA)	17.33	0.24	0.24
	assign (segid 3A4 and resid 305 and name CA)	(segid 3A4 and resid 384 and name CA)	18.28	0.36	0.36
	assign (segid 3A4 and resid 305 and name CA)	(segid 3A4 and resid 384 and name CB)	17.48	0.43	0.43
35	assign (segid 3A4 and resid 305 and name CA)	(segid 3A4 and resid 394 and name CA)	16.23	0.70	0.69
	assign (segid 3A4 and resid 305 and name CA)	(segid 3A4 and resid 394 and name CB)	16.50	0.72	0.73
	assign (segid 3A4 and resid 305 and name CA)	(segid 3A4 and resid 395 and name CA)	15.07	0.84	0.85
	assign (segid 3A4 and resid 305 and name CA)	(segid 3A4 and resid 396 and name CA)	15.59	0.68	0.69
	assign (segid 3A4 and resid 305 and name CA)	(segid 3A4 and resid 396 and name CB)	17.01	0.67	0.66
40	assign (segid 3A4 and resid 305 and name CA)	(segid 3A4 and resid 397 and name CA)	13.92	0.72	0.73
	assign (segid 3A4 and resid 305 and name CA)	(segid 3A4 and resid 397 and name CB)	14.43	0.72	0.73
	assign (segid 3A4 and resid 305 and name CA)	(segid 3A4 and resid 398 and name CA)	10.60	0.76	0.75
	assign (segid 3A4 and resid 305 and name CA)	(segid 3A4 and resid 398 and name CB)	10.58	0.79	0.79
	assign (segid 3A4 and resid 305 and name CA)	(segid 3A4 and resid 399 and name CA)	10.97	0.70	0.70
45	assign (segid 3A4 and resid 305 and name CA)	(segid 3A4 and resid 399 and name CB)	12.30	0.69	0.69
	assign (segid 3A4 and resid 305 and name CA)	(segid 3A4 and resid 400 and name CA)	11.99	0.73	0.74
	assign (segid 3A4 and resid 305 and name CA)	(segid 3A4 and resid 400 and name CB)	13.22	0.70	0.70
	assign (segid 3A4 and resid 305 and name CA)	(segid 3A4 and resid 401 and name CA)	9.28	0.64	0.65
	assign (segid 3A4 and resid 305 and name CA)	(segid 3A4 and resid 402 and name CA)	6.50	0.72	0.72
50	assign (segid 3A4 and resid 305 and name CA)	(segid 3A4 and resid 402 and name CB)	6.45	0.65	0.65
	assign (segid 3A4 and resid 305 and name CA)	(segid 3A4 and resid 403 and name CA)	9.25	0.75	0.75
	assign (segid 3A4 and resid 305 and name CA)	(segid 3A4 and resid 403 and name CB)	10.63	0.72	0.73
	assign (segid 3A4 and resid 305 and name CA)	(segid 3A4 and resid 404 and name CA)	10.35	0.92	0.92
	assign (segid 3A4 and resid 305 and name CA)	(segid 3A4 and resid 404 and name CB)	10.97	0.96	0.96
55	assign (segid 3A4 and resid 305 and name CA)	(segid 3A4 and resid 405 and name CA)	7.57	0.99	1.00
	assign (segid 3A4 and resid 305 and name CA)	(segid 3A4 and resid 405 and name CB)	6.54	0.93	0.93
	assign (segid 3A4 and resid 305 and name CA)	(segid 3A4 and resid 406 and name CA)	7.04	0.69	0.70
	assign (segid 3A4 and resid 305 and name CA)	(segid 3A4 and resid 407 and name CA)	10.79	0.68	0.68
	assign (segid 3A4 and resid 305 and name CA)	(segid 3A4 and resid 407 and name CB)	11.71	0.74	0.73
60	assign (segid 3A4 and resid 305 and name CA)	(segid 3A4 and resid 408 and name CA)	11.72	0.74	0.74
	assign (segid 3A4 and resid 305 and name CA)	(segid 3A4 and resid 408 and name CB)	11.56	0.85	0.84
	assign (segid 3A4 and resid 305 and name CA)	(segid 3A4 and resid 409 and name CA)	10.43	0.62	0.62
	assign (segid 3A4 and resid 305 and name CA)	(segid 3A4 and resid 409 and name CB)	9.21	0.75	0.75
	assign (segid 3A4 and resid 305 and name CA)	(segid 3A4 and resid 410 and name CA)	11.84	0.29	0.30
65	assign (segid 3A4 and resid 305 and name CA)	(segid 3A4 and resid 411 and name CA)	14.96	0.43	0.43
	assign (segid 3A4 and resid 305 and name CA)	(segid 3A4 and resid 411 and name CB)	15.31	0.58	0.58
	assign (segid 3A4 and resid 305 and name CA)	(segid 3A4 and resid 412 and name CA)	15.50	0.49	0.50
	assign (segid 3A4 and resid 305 and name CA)	(segid 3A4 and resid 413 and name CA)	17.02	1.02	1.02
	assign (segid 3A4 and resid 305 and name CB)	(segid 3A4 and resid 306 and name C)	5.49	0.06	0.06
70	assign (segid 3A4 and resid 305 and name CB)	(segid 3A4 and resid 306 and name CA)	4.54	0.07	0.07
	assign (segid 3A4 and resid 305 and name CB)	(segid 3A4 and resid 306 and name N)	3.21	0.05	0.06
	assign (segid 3A4 and resid 305 and name CB)	(segid 3A4 and resid 307 and name O)	6.36	0.06	0.07
	assign (segid 3A4 and resid 305 and name CB)	(segid 3A4 and resid 307 and name C)	6.84	0.06	0.05
	assign (segid 3A4 and resid 305 and name CB)	(segid 3A4 and resid 307 and name CA)	6.81	0.08	0.08
75	assign (segid 3A4 and resid 305 and name CB)	(segid 3A4 and resid 307 and name CB)	7.27	0.12	0.12
	assign (segid 3A4 and resid 305 and name CB)	(segid 3A4 and resid 307 and name N)	5.66	0.11	0.10
	assign (segid 3A4 and resid 305 and name CB)	(segid 3A4 and resid 307 and name O)	7.94	0.04	0.04
	assign (segid 3A4 and resid 305 and name CB)	(segid 3A4 and resid 308 and name C)	6.71	0.10	0.09
	assign (segid 3A4 and resid 305 and name CB)	(segid 3A4 and resid 308 and name CA)	6.24	0.10	0.09
80	assign (segid 3A4 and resid 305 and name CB)	(segid 3A4 and resid 308 and name CB)	5.37	0.16	0.16
	assign (segid 3A4 and resid 305 and name CB)	(segid 3A4 and resid 308 and name N)	5.85	0.08	0.08
	assign (segid 3A4 and resid 305 and name CB)	(segid 3A4 and resid 309 and name CA)	6.95	0.12	0.11

	assign (segid 3A4 and resid 305 and name CB)	(segid 3A4 and resid 309 and name CB)	6.50	0.16	0.16
	assign (segid 3A4 and resid 305 and name CB)	(segid 3A4 and resid 309 and name N)	6.10	0.07	0.06
	assign (segid 3A4 and resid 305 and name CB)	(segid 3A4 and resid 310 and name CA)	9.70	0.12	0.12
	assign (segid 3A4 and resid 305 and name CB)	(segid 3A4 and resid 310 and name CB)	9.85	0.21	0.20
5	assign (segid 3A4 and resid 305 and name CB)	(segid 3A4 and resid 311 and name CA)	11.04	0.13	0.12
	assign (segid 3A4 and resid 305 and name CB)	(segid 3A4 and resid 311 and name CB)	10.70	0.16	0.15
	assign (segid 3A4 and resid 305 and name CB)	(segid 3A4 and resid 312 and name CA)	11.28	0.19	0.19
	assign (segid 3A4 and resid 305 and name CB)	(segid 3A4 and resid 312 and name CB)	10.39	0.25	0.25
	assign (segid 3A4 and resid 305 and name CB)	(segid 3A4 and resid 313 and name CA)	13.21	0.22	0.21
10	assign (segid 3A4 and resid 305 and name CB)	(segid 3A4 and resid 313 and name CB)	12.87	0.25	0.25
	assign (segid 3A4 and resid 305 and name CB)	(segid 3A4 and resid 314 and name CA)	15.27	0.09	0.08
	assign (segid 3A4 and resid 305 and name CB)	(segid 3A4 and resid 314 and name CB)	15.01	0.08	0.09
	assign (segid 3A4 and resid 305 and name CB)	(segid 3A4 and resid 315 and name CA)	16.16	0.24	0.24
	assign (segid 3A4 and resid 305 and name CB)	(segid 3A4 and resid 315 and name CB)	15.41	0.31	0.32
15	assign (segid 3A4 and resid 305 and name CB)	(segid 3A4 and resid 316 and name CA)	16.96	0.37	0.37
	assign (segid 3A4 and resid 305 and name CB)	(segid 3A4 and resid 317 and name CA)	18.34	0.55	0.55
	assign (segid 3A4 and resid 305 and name CB)	(segid 3A4 and resid 318 and name CB)	18.59	0.74	0.74
	assign (segid 3A4 and resid 305 and name CB)	(segid 3A4 and resid 362 and name CA)	18.59	0.22	0.21
	assign (segid 3A4 and resid 305 and name CB)	(segid 3A4 and resid 362 and name CB)	18.96	0.20	0.21
20	assign (segid 3A4 and resid 305 and name CB)	(segid 3A4 and resid 363 and name CA)	14.93	0.25	0.24
	assign (segid 3A4 and resid 305 and name CB)	(segid 3A4 and resid 363 and name CB)	14.51	0.33	0.32
	assign (segid 3A4 and resid 305 and name CB)	(segid 3A4 and resid 364 and name CA)	13.46	0.20	0.20
	assign (segid 3A4 and resid 305 and name CB)	(segid 3A4 and resid 364 and name CB)	14.69	0.23	0.23
	assign (segid 3A4 and resid 305 and name CB)	(segid 3A4 and resid 365 and name CA)	9.96	0.27	0.26
25	assign (segid 3A4 and resid 305 and name CB)	(segid 3A4 and resid 365 and name CB)	8.79	0.20	0.21
	assign (segid 3A4 and resid 305 and name CB)	(segid 3A4 and resid 381 and name CA)	17.98	0.46	0.46
	assign (segid 3A4 and resid 305 and name CB)	(segid 3A4 and resid 383 and name CA)	18.03	0.27	0.27
	assign (segid 3A4 and resid 305 and name CB)	(segid 3A4 and resid 384 and name CA)	18.76	0.35	0.35
	assign (segid 3A4 and resid 305 and name CB)	(segid 3A4 and resid 384 and name CB)	17.91	0.40	0.41
30	assign (segid 3A4 and resid 305 and name CB)	(segid 3A4 and resid 394 and name CA)	16.23	0.68	0.69
	assign (segid 3A4 and resid 305 and name CB)	(segid 3A4 and resid 394 and name CB)	16.62	0.68	0.69
	assign (segid 3A4 and resid 305 and name CB)	(segid 3A4 and resid 395 and name CA)	14.84	0.84	0.83
	assign (segid 3A4 and resid 305 and name CB)	(segid 3A4 and resid 396 and name CA)	15.07	0.70	0.71
	assign (segid 3A4 and resid 305 and name CB)	(segid 3A4 and resid 396 and name CB)	16.46	0.68	0.68
35	assign (segid 3A4 and resid 305 and name CB)	(segid 3A4 and resid 397 and name CA)	13.59	0.74	0.75
	assign (segid 3A4 and resid 305 and name CB)	(segid 3A4 and resid 397 and name CB)	14.25	0.74	0.74
	assign (segid 3A4 and resid 305 and name CB)	(segid 3A4 and resid 398 and name CA)	10.37	0.76	0.75
	assign (segid 3A4 and resid 305 and name CB)	(segid 3A4 and resid 398 and name CB)	10.49	0.76	0.76
	assign (segid 3A4 and resid 305 and name CB)	(segid 3A4 and resid 399 and name CA)	10.25	0.73	0.72
40	assign (segid 3A4 and resid 305 and name CB)	(segid 3A4 and resid 399 and name CB)	11.53	0.70	0.71
	assign (segid 3A4 and resid 305 and name CB)	(segid 3A4 and resid 400 and name CA)	11.15	0.81	0.81
	assign (segid 3A4 and resid 305 and name CB)	(segid 3A4 and resid 400 and name CB)	12.45	0.79	0.78
	assign (segid 3A4 and resid 305 and name CB)	(segid 3A4 and resid 401 and name CA)	8.71	0.71	0.70
	assign (segid 3A4 and resid 305 and name CB)	(segid 3A4 and resid 402 and name C)	5.94	0.83	0.84
45	assign (segid 3A4 and resid 305 and name CB)	(segid 3A4 and resid 402 and name CA)	5.60	0.77	0.77
	assign (segid 3A4 and resid 305 and name CB)	(segid 3A4 and resid 402 and name CB)	5.62	0.67	0.68
	assign (segid 3A4 and resid 305 and name CB)	(segid 3A4 and resid 402 and name O)	5.30	0.87	0.87
	assign (segid 3A4 and resid 305 and name CB)	(segid 3A4 and resid 403 and name CA)	7.95	0.82	0.82
	assign (segid 3A4 and resid 305 and name CB)	(segid 3A4 and resid 403 and name CB)	9.36	0.80	0.79
50	assign (segid 3A4 and resid 305 and name CB)	(segid 3A4 and resid 404 and name CA)	9.22	0.98	0.99
	assign (segid 3A4 and resid 305 and name CB)	(segid 3A4 and resid 404 and name CB)	9.99	1.01	1.02
	assign (segid 3A4 and resid 305 and name CB)	(segid 3A4 and resid 405 and name CA)	6.66	1.05	1.04
	assign (segid 3A4 and resid 305 and name CB)	(segid 3A4 and resid 405 and name CB)	5.84	0.96	0.97
	assign (segid 3A4 and resid 305 and name CB)	(segid 3A4 and resid 406 and name CA)	5.69	0.70	0.71
55	assign (segid 3A4 and resid 305 and name CB)	(segid 3A4 and resid 406 and name N)	5.67	0.85	0.84
	assign (segid 3A4 and resid 305 and name CB)	(segid 3A4 and resid 407 and name CA)	9.43	0.68	0.68
	assign (segid 3A4 and resid 305 and name CB)	(segid 3A4 and resid 407 and name CB)	10.32	0.75	0.75
	assign (segid 3A4 and resid 305 and name CB)	(segid 3A4 and resid 408 and name CA)	10.67	0.74	0.73
	assign (segid 3A4 and resid 305 and name CB)	(segid 3A4 and resid 408 and name CB)	10.62	0.85	0.86
60	assign (segid 3A4 and resid 305 and name CB)	(segid 3A4 and resid 409 and name CA)	9.60	0.59	0.59
	assign (segid 3A4 and resid 305 and name CB)	(segid 3A4 and resid 409 and name CB)	8.50	0.77	0.77
	assign (segid 3A4 and resid 305 and name CB)	(segid 3A4 and resid 410 and name CA)	10.77	0.26	0.25
	assign (segid 3A4 and resid 305 and name CB)	(segid 3A4 and resid 411 and name CA)	13.86	0.35	0.35
	assign (segid 3A4 and resid 305 and name CB)	(segid 3A4 and resid 411 and name CB)	14.15	0.52	0.52
65	assign (segid 3A4 and resid 305 and name CB)	(segid 3A4 and resid 412 and name CA)	14.69	0.39	0.38
	assign (segid 3A4 and resid 305 and name CB)	(segid 3A4 and resid 413 and name CA)	16.60	0.97	0.97
	assign (segid 3A4 and resid 305 and name CB)	(segid 3A4 and resid 414 and name CA)	16.74	1.17	1.16
	assign (segid 3A4 and resid 305 and name N)	(segid 3A4 and resid 305 and name C)	2.49	0.04	0.03
	assign (segid 3A4 and resid 305 and name N)	(segid 3A4 and resid 305 and name CA)	1.46	0.01	0.01
70	assign (segid 3A4 and resid 305 and name N)	(segid 3A4 and resid 305 and name CB)	2.48	0.02	0.02
	assign (segid 3A4 and resid 305 and name N)	(segid 3A4 and resid 305 and name O)	3.50	0.03	0.04
	assign (segid 3A4 and resid 305 and name N)	(segid 3A4 and resid 306 and name C)	4.83	0.08	0.07
	assign (segid 3A4 and resid 305 and name N)	(segid 3A4 and resid 306 and name CA)	4.32	0.08	0.07
	assign (segid 3A4 and resid 305 and name N)	(segid 3A4 and resid 306 and name N)	2.90	0.07	0.07
75	assign (segid 3A4 and resid 305 and name N)	(segid 3A4 and resid 306 and name O)	5.93	0.07	0.07
	assign (segid 3A4 and resid 305 and name N)	(segid 3A4 and resid 307 and name C)	5.62	0.04	0.05
	assign (segid 3A4 and resid 305 and name N)	(segid 3A4 and resid 307 and name CA)	5.37	0.10	0.10
	assign (segid 3A4 and resid 305 and name N)	(segid 3A4 and resid 307 and name CB)	5.38	0.16	0.17
	assign (segid 3A4 and resid 305 and name N)	(segid 3A4 and resid 307 and name N)	4.41	0.11	0.11
80	assign (segid 3A4 and resid 305 and name N)	(segid 3A4 and resid 307 and name O)	6.83	0.05	0.04
	assign (segid 3A4 and resid 305 and name N)	(segid 3A4 and resid 308 and name C)	6.44	0.09	0.08
	assign (segid 3A4 and resid 305 and name N)	(segid 3A4 and resid 308 and name CA)	5.50	0.07	0.08
	assign (segid 3A4 and resid 305 and name N)	(segid 3A4 and resid 308 and name CB)	4.85	0.16	0.16

	assign (segid 3A4 and resid 305 and name N)	(segid 3A4 and resid 308 and name N)	4.77	0.04	0.03
	assign (segid 3A4 and resid 305 and name N)	(segid 3A4 and resid 308 and name O)	7.62	0.10	0.10
	assign (segid 3A4 and resid 305 and name N)	(segid 3A4 and resid 309 and name CA)	7.34	0.11	0.12
	assign (segid 3A4 and resid 305 and name N)	(segid 3A4 and resid 309 and name CB)	7.23	0.16	0.16
5	assign (segid 3A4 and resid 305 and name N)	(segid 3A4 and resid 309 and name N)	6.15	0.08	0.09
	assign (segid 3A4 and resid 305 and name N)	(segid 3A4 and resid 365 and name CB)	7.16	0.13	0.13
	assign (segid 3A4 and resid 305 and name N)	(segid 3A4 and resid 305 and name CB)	3.33	0.04	0.03
	assign (segid 3A4 and resid 305 and name O)	(segid 3A4 and resid 306 and name C)	2.94	0.09	0.08
	assign (segid 3A4 and resid 305 and name O)	(segid 3A4 and resid 306 and name CA)	2.76	0.03	0.02
	assign (segid 3A4 and resid 305 and name O)	(segid 3A4 and resid 306 and name N)	2.24	0.01	0.02
10	assign (segid 3A4 and resid 305 and name O)	(segid 3A4 and resid 306 and name O)	3.46	0.09	0.09
	assign (segid 3A4 and resid 305 and name O)	(segid 3A4 and resid 307 and name C)	3.94	0.11	0.11
	assign (segid 3A4 and resid 305 and name O)	(segid 3A4 and resid 307 and name CA)	4.24	0.15	0.15
	assign (segid 3A4 and resid 305 and name O)	(segid 3A4 and resid 307 and name CB)	5.18	0.15	0.15
	assign (segid 3A4 and resid 305 and name O)	(segid 3A4 and resid 307 and name N)	3.32	0.16	0.15
15	assign (segid 3A4 and resid 305 and name O)	(segid 3A4 and resid 307 and name O)	4.90	0.08	0.07
	assign (segid 3A4 and resid 305 and name O)	(segid 3A4 and resid 308 and name C)	3.66	0.04	0.04
	assign (segid 3A4 and resid 305 and name O)	(segid 3A4 and resid 308 and name CA)	3.51	0.08	0.08
	assign (segid 3A4 and resid 305 and name O)	(segid 3A4 and resid 308 and name CB)	3.32	0.07	0.06
	assign (segid 3A4 and resid 305 and name O)	(segid 3A4 and resid 308 and name N)	3.06	0.13	0.14
20	assign (segid 3A4 and resid 305 and name O)	(segid 3A4 and resid 308 and name O)	4.85	0.05	0.06
	assign (segid 3A4 and resid 305 and name O)	(segid 3A4 and resid 309 and name C)	5.05	0.06	0.05
	assign (segid 3A4 and resid 305 and name O)	(segid 3A4 and resid 309 and name CA)	3.90	0.11	0.12
	assign (segid 3A4 and resid 305 and name O)	(segid 3A4 and resid 309 and name CB)	3.76	0.18	0.18
	assign (segid 3A4 and resid 305 and name O)	(segid 3A4 and resid 309 and name N)	2.92	0.05	0.05
25	assign (segid 3A4 and resid 305 and name O)	(segid 3A4 and resid 309 and name O)	6.17	0.07	0.08
	assign (segid 3A4 and resid 305 and name O)	(segid 3A4 and resid 310 and name C)	7.21	0.06	0.05
	assign (segid 3A4 and resid 305 and name O)	(segid 3A4 and resid 310 and name CA)	6.42	0.07	0.07
	assign (segid 3A4 and resid 305 and name O)	(segid 3A4 and resid 310 and name CB)	6.66	0.15	0.14
	assign (segid 3A4 and resid 305 and name O)	(segid 3A4 and resid 310 and name N)	5.06	0.06	0.05
30	assign (segid 3A4 and resid 305 and name O)	(segid 3A4 and resid 311 and name CB)	7.68	0.13	0.14
	assign (segid 3A4 and resid 305 and name O)	(segid 3A4 and resid 311 and name N)	6.80	0.07	0.08
	assign (segid 3A4 and resid 305 and name O)	(segid 3A4 and resid 312 and name CB)	7.68	0.17	0.16
	assign (segid 3A4 and resid 305 and name O)	(segid 3A4 and resid 312 and name N)	7.58	0.05	0.05
	assign (segid 3A4 and resid 305 and name O)	(segid 3A4 and resid 365 and name CB)	6.98	0.15	0.14
35	assign (segid 3A4 and resid 305 and name O)	(segid 3A4 and resid 402 and name CA)	5.92	0.56	0.56
	assign (segid 3A4 and resid 305 and name O)	(segid 3A4 and resid 402 and name CB)	5.90	0.53	0.53
	assign (segid 3A4 and resid 305 and name O)	(segid 3A4 and resid 402 and name N)	6.59	0.56	0.55
	assign (segid 3A4 and resid 305 and name O)	(segid 3A4 and resid 402 and name O)	6.81	0.52	0.52
	assign (segid 3A4 and resid 305 and name O)	(segid 3A4 and resid 405 and name CB)	6.40	0.63	0.62
40	assign (segid 3A4 and resid 306 and name C)	(segid 3A4 and resid 306 and name O)	1.24	0.01	0.01
	assign (segid 3A4 and resid 306 and name C)	(segid 3A4 and resid 307 and name C)	3.06	0.07	0.07
	assign (segid 3A4 and resid 306 and name C)	(segid 3A4 and resid 307 and name CA)	2.44	0.01	0.02
	assign (segid 3A4 and resid 306 and name C)	(segid 3A4 and resid 307 and name CB)	3.70	0.01	0.01
	assign (segid 3A4 and resid 306 and name C)	(segid 3A4 and resid 307 and name N)	1.32	0.01	0.02
45	assign (segid 3A4 and resid 306 and name C)	(segid 3A4 and resid 307 and name O)	3.94	0.10	0.11
	assign (segid 3A4 and resid 306 and name C)	(segid 3A4 and resid 308 and name C)	4.53	0.05	0.04
	assign (segid 3A4 and resid 306 and name C)	(segid 3A4 and resid 308 and name CA)	4.45	0.06	0.07
	assign (segid 3A4 and resid 306 and name C)	(segid 3A4 and resid 308 and name CB)	5.17	0.06	0.05
	assign (segid 3A4 and resid 306 and name C)	(segid 3A4 and resid 308 and name N)	3.29	0.07	0.06
50	assign (segid 3A4 and resid 306 and name C)	(segid 3A4 and resid 308 and name O)	5.58	0.08	0.08
	assign (segid 3A4 and resid 306 and name C)	(segid 3A4 and resid 309 and name C)	4.88	0.04	0.05
	assign (segid 3A4 and resid 306 and name C)	(segid 3A4 and resid 309 and name CA)	4.55	0.09	0.09
	assign (segid 3A4 and resid 306 and name C)	(segid 3A4 and resid 309 and name CB)	4.33	0.19	0.19
	assign (segid 3A4 and resid 306 and name C)	(segid 3A4 and resid 309 and name N)	3.81	0.06	0.07
55	assign (segid 3A4 and resid 306 and name C)	(segid 3A4 and resid 309 and name O)	6.09	0.05	0.06
	assign (segid 3A4 and resid 306 and name C)	(segid 3A4 and resid 310 and name C)	6.17	0.13	0.13
	assign (segid 3A4 and resid 306 and name C)	(segid 3A4 and resid 310 and name CA)	5.10	0.15	0.15
	assign (segid 3A4 and resid 306 and name C)	(segid 3A4 and resid 310 and name CB)	4.71	0.23	0.24
	assign (segid 3A4 and resid 306 and name C)	(segid 3A4 and resid 310 and name N)	4.16	0.08	0.08
60	assign (segid 3A4 and resid 306 and name C)	(segid 3A4 and resid 310 and name O)	7.34	0.14	0.15
	assign (segid 3A4 and resid 306 and name C)	(segid 3A4 and resid 311 and name CA)	7.31	0.12	0.11
	assign (segid 3A4 and resid 306 and name C)	(segid 3A4 and resid 311 and name CB)	7.33	0.12	0.13
	assign (segid 3A4 and resid 306 and name C)	(segid 3A4 and resid 311 and name N)	6.02	0.11	0.12
	assign (segid 3A4 and resid 306 and name C)	(segid 3A4 and resid 312 and name N)	7.80	0.08	0.09
65	assign (segid 3A4 and resid 306 and name C)	(segid 3A4 and resid 365 and name CB)	7.36	0.34	0.34
	assign (segid 3A4 and resid 306 and name C)	(segid 3A4 and resid 365 and name O)	6.84	0.15	0.15
	assign (segid 3A4 and resid 306 and name C)	(segid 3A4 and resid 306 and name C)	1.52	0.01	0.01
	assign (segid 3A4 and resid 306 and name CA)	(segid 3A4 and resid 306 and name O)	2.40	0.03	0.02
	assign (segid 3A4 and resid 306 and name CA)	(segid 3A4 and resid 307 and name C)	4.41	0.06	0.06
70	assign (segid 3A4 and resid 306 and name CA)	(segid 3A4 and resid 307 and name CA)	3.80	0.00	0.01
	assign (segid 3A4 and resid 306 and name CA)	(segid 3A4 and resid 307 and name CB)	4.83	0.03	0.02
	assign (segid 3A4 and resid 306 and name CA)	(segid 3A4 and resid 307 and name N)	2.42	0.01	0.02
	assign (segid 3A4 and resid 306 and name CA)	(segid 3A4 and resid 307 and name O)	5.38	0.10	0.10
	assign (segid 3A4 and resid 306 and name CA)	(segid 3A4 and resid 308 and name C)	5.43	0.06	0.06
75	assign (segid 3A4 and resid 306 and name CA)	(segid 3A4 and resid 308 and name CA)	5.37	0.06	0.06
	assign (segid 3A4 and resid 306 and name CA)	(segid 3A4 and resid 308 and name CB)	5.71	0.05	0.06
	assign (segid 3A4 and resid 306 and name CA)	(segid 3A4 and resid 308 and name N)	4.32	0.05	0.05
	assign (segid 3A4 and resid 306 and name CA)	(segid 3A4 and resid 308 and name O)	6.55	0.08	0.09
	assign (segid 3A4 and resid 306 and name CA)	(segid 3A4 and resid 309 and name C)	5.75	0.10	0.09
80	assign (segid 3A4 and resid 306 and name CA)	(segid 3A4 and resid 309 and name CA)	5.13	0.08	0.07
	assign (segid 3A4 and resid 306 and name CA)	(segid 3A4 and resid 309 and name CB)	4.51	0.16	0.16
	assign (segid 3A4 and resid 306 and name CA)	(segid 3A4 and resid 309 and name N)	4.52	0.05	0.05

	assign (segid 3A4 and resid 306 and name CA)	(segid 3A4 and resid 309 and name O)	6.94	0.10	0.09
	assign (segid 3A4 and resid 306 and name CA)	(segid 3A4 and resid 310 and name C)	7.46	0.16	0.16
	assign (segid 3A4 and resid 306 and name CA)	(segid 3A4 and resid 310 and name CA)	6.29	0.19	0.19
	assign (segid 3A4 and resid 306 and name CA)	(segid 3A4 and resid 310 and name CB)	6.02	0.26	0.25
5	assign (segid 3A4 and resid 306 and name CA)	(segid 3A4 and resid 310 and name N)	5.24	0.13	0.14
	assign (segid 3A4 and resid 306 and name CA)	(segid 3A4 and resid 311 and name CA)	8.67	0.12	0.12
	assign (segid 3A4 and resid 306 and name CA)	(segid 3A4 and resid 311 and name CB)	8.71	0.12	0.13
	assign (segid 3A4 and resid 306 and name CA)	(segid 3A4 and resid 311 and name N)	7.38	0.13	0.13
	assign (segid 3A4 and resid 306 and name CA)	(segid 3A4 and resid 312 and name CA)	9.41	0.14	0.14
10	assign (segid 3A4 and resid 306 and name CA)	(segid 3A4 and resid 312 and name CB)	9.41	0.14	0.14
	assign (segid 3A4 and resid 306 and name CA)	(segid 3A4 and resid 313 and name CA)	10.80	0.17	0.17
	assign (segid 3A4 and resid 306 and name CA)	(segid 3A4 and resid 313 and name CB)	10.13	0.22	0.22
	assign (segid 3A4 and resid 306 and name CA)	(segid 3A4 and resid 314 and name CA)	12.47	0.13	0.12
	assign (segid 3A4 and resid 306 and name CA)	(segid 3A4 and resid 314 and name CB)	12.09	0.18	0.18
	assign (segid 3A4 and resid 306 and name CA)	(segid 3A4 and resid 315 and name CA)	14.27	0.16	0.16
15	assign (segid 3A4 and resid 306 and name CA)	(segid 3A4 and resid 315 and name CB)	13.86	0.24	0.24
	assign (segid 3A4 and resid 306 and name CA)	(segid 3A4 and resid 316 and name CA)	15.42	0.26	0.25
	assign (segid 3A4 and resid 306 and name CA)	(segid 3A4 and resid 317 and name CA)	16.08	0.55	0.54
	assign (segid 3A4 and resid 306 and name CA)	(segid 3A4 and resid 318 and name CA)	17.64	0.69	0.69
	assign (segid 3A4 and resid 306 and name CA)	(segid 3A4 and resid 318 and name CB)	16.95	0.73	0.73
20	assign (segid 3A4 and resid 306 and name CA)	(segid 3A4 and resid 318 and name N)	19.60	0.38	0.37
	assign (segid 3A4 and resid 306 and name CA)	(segid 3A4 and resid 347 and name CA)	17.30	0.35	0.35
	assign (segid 3A4 and resid 306 and name CA)	(segid 3A4 and resid 351 and name CA)	17.90	0.68	0.69
	assign (segid 3A4 and resid 306 and name CA)	(segid 3A4 and resid 357 and name CA)	17.05	0.68	0.68
	assign (segid 3A4 and resid 306 and name CA)	(segid 3A4 and resid 357 and name CB)	18.59	0.32	0.33
25	assign (segid 3A4 and resid 306 and name CA)	(segid 3A4 and resid 360 and name CA)	19.46	0.36	0.35
	assign (segid 3A4 and resid 306 and name CA)	(segid 3A4 and resid 360 and name CB)	19.44	0.23	0.23
	assign (segid 3A4 and resid 306 and name CA)	(segid 3A4 and resid 361 and name CA)	17.52	0.20	0.21
	assign (segid 3A4 and resid 306 and name CA)	(segid 3A4 and resid 362 and name CA)	17.91	0.25	0.25
	assign (segid 3A4 and resid 306 and name CA)	(segid 3A4 and resid 362 and name CB)	14.16	0.22	0.22
30	assign (segid 3A4 and resid 306 and name CA)	(segid 3A4 and resid 363 and name CA)	14.09	0.28	0.28
	assign (segid 3A4 and resid 306 and name CA)	(segid 3A4 and resid 363 and name CB)	12.54	0.14	0.13
	assign (segid 3A4 and resid 306 and name CA)	(segid 3A4 and resid 364 and name CA)	13.58	0.12	0.11
	assign (segid 3A4 and resid 306 and name CA)	(segid 3A4 and resid 364 and name CB)	8.94	0.17	0.17
	assign (segid 3A4 and resid 306 and name CA)	(segid 3A4 and resid 365 and name CA)	8.40	0.26	0.25
35	assign (segid 3A4 and resid 306 and name CA)	(segid 3A4 and resid 365 and name CB)	14.09	0.52	0.53
	assign (segid 3A4 and resid 306 and name CA)	(segid 3A4 and resid 381 and name CA)	16.13	0.32	0.32
	assign (segid 3A4 and resid 306 and name CA)	(segid 3A4 and resid 382 and name CA)	17.62	0.34	0.34
	assign (segid 3A4 and resid 306 and name CA)	(segid 3A4 and resid 382 and name CB)	14.71	0.28	0.28
	assign (segid 3A4 and resid 306 and name CA)	(segid 3A4 and resid 383 and name CA)	15.30	0.35	0.35
40	assign (segid 3A4 and resid 306 and name CA)	(segid 3A4 and resid 384 and name CA)	14.37	0.42	0.41
	assign (segid 3A4 and resid 306 and name CA)	(segid 3A4 and resid 384 and name CB)	18.55	0.24	0.25
	assign (segid 3A4 and resid 306 and name CA)	(segid 3A4 and resid 385 and name CA)	17.88	0.63	0.62
	assign (segid 3A4 and resid 306 and name CA)	(segid 3A4 and resid 391 and name CA)	16.70	0.60	0.59
	assign (segid 3A4 and resid 306 and name CA)	(segid 3A4 and resid 391 and name CB)	16.41	0.71	0.70
45	assign (segid 3A4 and resid 306 and name CA)	(segid 3A4 and resid 393 and name CA)	13.19	0.75	0.74
	assign (segid 3A4 and resid 306 and name CA)	(segid 3A4 and resid 394 and name CA)	13.26	0.77	0.77
	assign (segid 3A4 and resid 306 and name CA)	(segid 3A4 and resid 394 and name CB)	12.06	0.88	0.88
	assign (segid 3A4 and resid 306 and name CA)	(segid 3A4 and resid 395 and name CA)	13.31	0.69	0.68
	assign (segid 3A4 and resid 306 and name CA)	(segid 3A4 and resid 396 and name CA)	14.79	0.67	0.67
50	assign (segid 3A4 and resid 306 and name CA)	(segid 3A4 and resid 396 and name CB)	11.84	0.71	0.70
	assign (segid 3A4 and resid 306 and name CA)	(segid 3A4 and resid 397 and name CA)	12.21	0.72	0.71
	assign (segid 3A4 and resid 306 and name CA)	(segid 3A4 and resid 397 and name CB)	8.17	0.74	0.74
	assign (segid 3A4 and resid 306 and name CA)	(segid 3A4 and resid 398 and name CA)	7.71	0.81	0.81
	assign (segid 3A4 and resid 306 and name CA)	(segid 3A4 and resid 398 and name CB)	9.24	0.67	0.68
55	assign (segid 3A4 and resid 306 and name CA)	(segid 3A4 and resid 399 and name CA)	10.50	0.69	0.69
	assign (segid 3A4 and resid 306 and name CA)	(segid 3A4 and resid 399 and name CB)	11.18	0.62	0.62
	assign (segid 3A4 and resid 306 and name CA)	(segid 3A4 and resid 400 and name CA)	12.31	0.59	0.59
	assign (segid 3A4 and resid 306 and name CA)	(segid 3A4 and resid 400 and name CB)	8.82	0.45	0.46
60	assign (segid 3A4 and resid 306 and name CA)	(segid 3A4 and resid 401 and name CA)	6.39	0.52	0.52
	assign (segid 3A4 and resid 306 and name CA)	(segid 3A4 and resid 402 and name CA)	5.69	0.54	0.53
	assign (segid 3A4 and resid 306 and name CA)	(segid 3A4 and resid 402 and name CB)	9.83	0.50	0.51
	assign (segid 3A4 and resid 306 and name CA)	(segid 3A4 and resid 403 and name CA)	10.89	0.51	0.52
	assign (segid 3A4 and resid 306 and name CA)	(segid 3A4 and resid 403 and name CB)	11.55	0.59	0.59
	assign (segid 3A4 and resid 306 and name CA)	(segid 3A4 and resid 404 and name CA)	11.93	0.64	0.63
65	assign (segid 3A4 and resid 306 and name CA)	(segid 3A4 and resid 404 and name CB)	9.65	0.58	0.58
	assign (segid 3A4 and resid 306 and name CA)	(segid 3A4 and resid 405 and name CA)	8.50	0.51	0.51
	assign (segid 3A4 and resid 306 and name CA)	(segid 3A4 and resid 405 and name CB)	9.59	0.44	0.43
	assign (segid 3A4 and resid 306 and name CA)	(segid 3A4 and resid 406 and name CA)	13.20	0.41	0.40
	assign (segid 3A4 and resid 306 and name CA)	(segid 3A4 and resid 407 and name CA)	13.79	0.45	0.46
70	assign (segid 3A4 and resid 306 and name CA)	(segid 3A4 and resid 407 and name CB)	14.43	0.46	0.46
	assign (segid 3A4 and resid 306 and name CA)	(segid 3A4 and resid 408 and name CA)	14.13	0.55	0.55
	assign (segid 3A4 and resid 306 and name CA)	(segid 3A4 and resid 408 and name CB)	13.78	0.55	0.56
	assign (segid 3A4 and resid 306 and name CA)	(segid 3A4 and resid 409 and name CA)	12.66	0.73	0.72
	assign (segid 3A4 and resid 306 and name CA)	(segid 3A4 and resid 409 and name CB)	15.19	0.33	0.33
75	assign (segid 3A4 and resid 306 and name CA)	(segid 3A4 and resid 410 and name CA)	18.15	0.31	0.31
	assign (segid 3A4 and resid 306 and name CA)	(segid 3A4 and resid 411 and name CA)	18.31	0.43	0.41
	assign (segid 3A4 and resid 306 and name CA)	(segid 3A4 and resid 411 and name CB)	18.86	0.40	0.40
	assign (segid 3A4 and resid 306 and name CA)	(segid 3A4 and resid 412 and name CA)	2.48	0.02	0.02
80	assign (segid 3A4 and resid 306 and name N)	(segid 3A4 and resid 306 and name C)	1.47	0.01	0.01
	assign (segid 3A4 and resid 306 and name N)	(segid 3A4 and resid 306 and name O)	3.53	0.03	0.03
	assign (segid 3A4 and resid 306 and name N)	(segid 3A4 and resid 307 and name C)	4.67	0.05	0.04
	assign (segid 3A4 and resid 306 and name N)	(segid 3A4 and resid 307 and name CA)	4.19	0.05	0.05

	assign (segid 3A4 and resid 306 and name N)	(segid 3A4 and resid 307 and name CB)	4.91	0.09	0.08
	assign (segid 3A4 and resid 306 and name N)	(segid 3A4 and resid 307 and name N)	2.80	0.06	0.06
	assign (segid 3A4 and resid 306 and name N)	(segid 3A4 and resid 307 and name O)	5.79	0.07	0.07
	assign (segid 3A4 and resid 306 and name N)	(segid 3A4 and resid 308 and name C)	5.55	0.06	0.06
	assign (segid 3A4 and resid 306 and name N)	(segid 3A4 and resid 308 and name CA)	5.20	0.05	0.05
5	assign (segid 3A4 and resid 306 and name N)	(segid 3A4 and resid 308 and name CB)	5.17	0.09	0.09
	assign (segid 3A4 and resid 306 and name N)	(segid 3A4 and resid 308 and name N)	4.22	0.04	0.03
	assign (segid 3A4 and resid 306 and name N)	(segid 3A4 and resid 308 and name O)	6.75	0.06	0.07
	assign (segid 3A4 and resid 306 and name N)	(segid 3A4 and resid 309 and name C)	6.51	0.08	0.07
	assign (segid 3A4 and resid 306 and name N)	(segid 3A4 and resid 309 and name CA)	5.64	0.10	0.09
10	assign (segid 3A4 and resid 306 and name N)	(segid 3A4 and resid 309 and name CB)	5.15	0.17	0.16
	assign (segid 3A4 and resid 306 and name N)	(segid 3A4 and resid 309 and name N)	4.79	0.08	0.07
	assign (segid 3A4 and resid 306 and name N)	(segid 3A4 and resid 309 and name O)	7.70	0.08	0.08
	assign (segid 3A4 and resid 306 and name N)	(segid 3A4 and resid 310 and name CA)	7.33	0.16	0.15
	assign (segid 3A4 and resid 306 and name N)	(segid 3A4 and resid 310 and name CB)	7.14	0.23	0.22
15	assign (segid 3A4 and resid 306 and name N)	(segid 3A4 and resid 310 and name N)	6.16	0.11	0.11
	assign (segid 3A4 and resid 306 and name N)	(segid 3A4 and resid 402 and name CA)	6.29	0.63	0.63
	assign (segid 3A4 and resid 306 and name N)	(segid 3A4 and resid 402 and name CB)	5.75	0.63	0.63
	assign (segid 3A4 and resid 306 and name N)	(segid 3A4 and resid 307 and name C)	3.08	0.11	0.12
	assign (segid 3A4 and resid 306 and name O)	(segid 3A4 and resid 307 and name CA)	2.81	0.05	0.04
20	assign (segid 3A4 and resid 306 and name O)	(segid 3A4 and resid 307 and name CB)	4.27	0.04	0.04
	assign (segid 3A4 and resid 306 and name O)	(segid 3A4 and resid 307 and name N)	2.25	0.01	0.01
	assign (segid 3A4 and resid 306 and name O)	(segid 3A4 and resid 307 and name O)	3.62	0.16	0.16
	assign (segid 3A4 and resid 306 and name O)	(segid 3A4 and resid 308 and name C)	4.17	0.09	0.10
	assign (segid 3A4 and resid 306 and name O)	(segid 3A4 and resid 308 and name CA)	4.48	0.12	0.11
25	assign (segid 3A4 and resid 306 and name O)	(segid 3A4 and resid 308 and name CB)	5.41	0.11	0.11
	assign (segid 3A4 and resid 306 and name O)	(segid 3A4 and resid 308 and name N)	3.53	0.11	0.10
	assign (segid 3A4 and resid 306 and name O)	(segid 3A4 and resid 308 and name O)	5.06	0.12	0.12
	assign (segid 3A4 and resid 306 and name O)	(segid 3A4 and resid 309 and name C)	3.88	0.04	0.04
	assign (segid 3A4 and resid 306 and name O)	(segid 3A4 and resid 309 and name CA)	3.81	0.13	0.13
30	assign (segid 3A4 and resid 306 and name O)	(segid 3A4 and resid 309 and name CB)	3.64	0.25	0.25
	assign (segid 3A4 and resid 306 and name O)	(segid 3A4 and resid 309 and name N)	3.38	0.13	0.12
	assign (segid 3A4 and resid 306 and name O)	(segid 3A4 and resid 309 and name O)	5.05	0.06	0.05
	assign (segid 3A4 and resid 306 and name O)	(segid 3A4 and resid 310 and name C)	5.13	0.17	0.17
	assign (segid 3A4 and resid 306 and name O)	(segid 3A4 and resid 310 and name CA)	3.95	0.18	0.18
35	assign (segid 3A4 and resid 306 and name O)	(segid 3A4 and resid 310 and name CB)	3.66	0.27	0.26
	assign (segid 3A4 and resid 306 and name O)	(segid 3A4 and resid 310 and name N)	3.05	0.09	0.10
	assign (segid 3A4 and resid 306 and name O)	(segid 3A4 and resid 310 and name O)	6.26	0.18	0.18
	assign (segid 3A4 and resid 306 and name O)	(segid 3A4 and resid 311 and name C)	7.34	0.11	0.12
40	assign (segid 3A4 and resid 306 and name O)	(segid 3A4 and resid 311 and name CA)	6.53	0.15	0.15
	assign (segid 3A4 and resid 306 and name O)	(segid 3A4 and resid 311 and name CB)	6.79	0.16	0.15
	assign (segid 3A4 and resid 306 and name O)	(segid 3A4 and resid 311 and name N)	5.16	0.15	0.16
	assign (segid 3A4 and resid 306 and name O)	(segid 3A4 and resid 312 and name N)	6.99	0.11	0.10
	assign (segid 3A4 and resid 306 and name O)	(segid 3A4 and resid 365 and name O)	7.07	0.16	0.16
	assign (segid 3A4 and resid 306 and name O)	(segid 3A4 and resid 402 and name CB)	7.04	0.42	0.43
45	assign (segid 3A4 and resid 307 and name C)	(segid 3A4 and resid 307 and name CB)	2.48	0.02	0.03
	assign (segid 3A4 and resid 307 and name C)	(segid 3A4 and resid 307 and name O)	1.24	0.02	0.01
	assign (segid 3A4 and resid 307 and name C)	(segid 3A4 and resid 308 and name C)	3.02	0.02	0.03
	assign (segid 3A4 and resid 307 and name C)	(segid 3A4 and resid 308 and name CA)	2.45	0.02	0.01
	assign (segid 3A4 and resid 307 and name C)	(segid 3A4 and resid 308 and name CB)	3.73	0.03	0.03
50	assign (segid 3A4 and resid 307 and name C)	(segid 3A4 and resid 308 and name N)	1.34	0.01	0.00
	assign (segid 3A4 and resid 307 and name C)	(segid 3A4 and resid 308 and name O)	3.82	0.06	0.06
	assign (segid 3A4 and resid 307 and name C)	(segid 3A4 and resid 309 and name C)	4.55	0.06	0.05
	assign (segid 3A4 and resid 307 and name C)	(segid 3A4 and resid 309 and name CA)	4.51	0.09	0.10
	assign (segid 3A4 and resid 307 and name C)	(segid 3A4 and resid 309 and name CB)	5.28	0.15	0.14
55	assign (segid 3A4 and resid 307 and name C)	(segid 3A4 and resid 309 and name N)	3.34	0.11	0.11
	assign (segid 3A4 and resid 307 and name C)	(segid 3A4 and resid 309 and name O)	5.60	0.05	0.05
	assign (segid 3A4 and resid 307 and name C)	(segid 3A4 and resid 310 and name C)	4.84	0.10	0.11
	assign (segid 3A4 and resid 307 and name C)	(segid 3A4 and resid 310 and name CA)	4.52	0.11	0.11
	assign (segid 3A4 and resid 307 and name C)	(segid 3A4 and resid 310 and name CB)	4.29	0.16	0.17
60	assign (segid 3A4 and resid 307 and name C)	(segid 3A4 and resid 310 and name N)	3.81	0.08	0.08
	assign (segid 3A4 and resid 307 and name C)	(segid 3A4 and resid 310 and name O)	6.06	0.11	0.11
	assign (segid 3A4 and resid 307 and name C)	(segid 3A4 and resid 311 and name C)	6.05	0.06	0.07
	assign (segid 3A4 and resid 307 and name C)	(segid 3A4 and resid 311 and name CA)	5.02	0.10	0.11
	assign (segid 3A4 and resid 307 and name C)	(segid 3A4 and resid 311 and name CB)	4.61	0.10	0.10
65	assign (segid 3A4 and resid 307 and name C)	(segid 3A4 and resid 311 and name CD)	6.96	0.14	0.14
	assign (segid 3A4 and resid 307 and name C)	(segid 3A4 and resid 311 and name CG)	5.97	0.10	0.10
	assign (segid 3A4 and resid 307 and name C)	(segid 3A4 and resid 311 and name N)	4.10	0.10	0.11
	assign (segid 3A4 and resid 307 and name C)	(segid 3A4 and resid 311 and name O)	7.23	0.08	0.09
	assign (segid 3A4 and resid 307 and name C)	(segid 3A4 and resid 311 and name OE1)	6.88	0.18	0.19
70	assign (segid 3A4 and resid 307 and name C)	(segid 3A4 and resid 312 and name CA)	7.22	0.06	0.07
	assign (segid 3A4 and resid 307 and name C)	(segid 3A4 and resid 312 and name CB)	7.28	0.12	0.12
	assign (segid 3A4 and resid 307 and name C)	(segid 3A4 and resid 312 and name N)	5.95	0.06	0.06
	assign (segid 3A4 and resid 307 and name C)	(segid 3A4 and resid 313 and name N)	7.86	0.08	0.07
	assign (segid 3A4 and resid 307 and name C)	(segid 3A4 and resid 364 and name O)	6.79	0.12	0.13
75	assign (segid 3A4 and resid 307 and name C)	(segid 3A4 and resid 364 and name CA)	6.53	0.14	0.13
	assign (segid 3A4 and resid 307 and name C)	(segid 3A4 and resid 365 and name C)	5.00	0.19	0.19
	assign (segid 3A4 and resid 307 and name C)	(segid 3A4 and resid 365 and name CA)	4.79	0.24	0.25
	assign (segid 3A4 and resid 307 and name C)	(segid 3A4 and resid 365 and name CB)	4.63	0.40	0.40
	assign (segid 3A4 and resid 307 and name C)	(segid 3A4 and resid 365 and name N)	6.10	0.24	0.24
80	assign (segid 3A4 and resid 307 and name C)	(segid 3A4 and resid 365 and name O)	4.29	0.24	0.24
	assign (segid 3A4 and resid 307 and name CA)	(segid 3A4 and resid 307 and name C)	1.51	0.01	0.02
	assign (segid 3A4 and resid 307 and name CA)	(segid 3A4 and resid 307 and name CB)	1.52	0.01	0.01

	assign (segid 3A4 and resid 307 and name CA) (segid 3A4 and resid 307 and name O)	2.40	0.03	0.03
	assign (segid 3A4 and resid 307 and name CA) (segid 3A4 and resid 308 and name C)	4.39	0.04	0.04
	assign (segid 3A4 and resid 307 and name CA) (segid 3A4 and resid 308 and name CA)	3.80	0.01	0.02
	assign (segid 3A4 and resid 307 and name CA) (segid 3A4 and resid 308 and name CB)	4.86	0.05	0.05
5	assign (segid 3A4 and resid 307 and name CA) (segid 3A4 and resid 308 and name N)	2.43	0.02	0.02
	assign (segid 3A4 and resid 307 and name CA) (segid 3A4 and resid 308 and name O)	5.26	0.05	0.05
	assign (segid 3A4 and resid 307 and name CA) (segid 3A4 and resid 309 and name C)	5.46	0.10	0.09
	assign (segid 3A4 and resid 307 and name CA) (segid 3A4 and resid 309 and name CA)	5.46	0.14	0.13
	assign (segid 3A4 and resid 307 and name CA) (segid 3A4 and resid 309 and name CB)	5.88	0.21	0.20
	assign (segid 3A4 and resid 307 and name CA) (segid 3A4 and resid 309 and name N)	4.39	0.14	0.13
10	assign (segid 3A4 and resid 307 and name CA) (segid 3A4 and resid 309 and name O)	6.57	0.09	0.09
	assign (segid 3A4 and resid 307 and name CA) (segid 3A4 and resid 310 and name C)	5.68	0.10	0.10
	assign (segid 3A4 and resid 307 and name CA) (segid 3A4 and resid 310 and name CA)	5.08	0.12	0.13
	assign (segid 3A4 and resid 307 and name CA) (segid 3A4 and resid 310 and name CB)	4.45	0.19	0.19
	assign (segid 3A4 and resid 307 and name CA) (segid 3A4 and resid 310 and name N)	4.52	0.10	0.09
15	assign (segid 3A4 and resid 307 and name CA) (segid 3A4 and resid 310 and name O)	6.87	0.11	0.11
	assign (segid 3A4 and resid 307 and name CA) (segid 3A4 and resid 311 and name C)	7.33	0.05	0.05
	assign (segid 3A4 and resid 307 and name CA) (segid 3A4 and resid 311 and name CA)	6.18	0.08	0.09
	assign (segid 3A4 and resid 307 and name CA) (segid 3A4 and resid 311 and name CB)	5.84	0.08	0.08
20	assign (segid 3A4 and resid 307 and name CA) (segid 3A4 and resid 311 and name CG)	7.20	0.11	0.11
	assign (segid 3A4 and resid 307 and name CA) (segid 3A4 and resid 311 and name N)	5.16	0.09	0.08
	assign (segid 3A4 and resid 307 and name CA) (segid 3A4 and resid 312 and name CA)	8.59	0.07	0.08
	assign (segid 3A4 and resid 307 and name CA) (segid 3A4 and resid 312 and name CB)	8.65	0.14	0.15
	assign (segid 3A4 and resid 307 and name CA) (segid 3A4 and resid 312 and name N)	7.29	0.07	0.08
25	assign (segid 3A4 and resid 307 and name CA) (segid 3A4 and resid 313 and name CA)	9.99	0.14	0.13
	assign (segid 3A4 and resid 307 and name CA) (segid 3A4 and resid 313 and name CB)	9.63	0.20	0.21
	assign (segid 3A4 and resid 307 and name CA) (segid 3A4 and resid 314 and name CA)	10.54	0.12	0.12
	assign (segid 3A4 and resid 307 and name CA) (segid 3A4 and resid 314 and name CB)	9.79	0.16	0.16
	assign (segid 3A4 and resid 307 and name CA) (segid 3A4 and resid 314 and name N)	12.15	0.21	0.21
30	assign (segid 3A4 and resid 307 and name CA) (segid 3A4 and resid 315 and name CB)	11.65	0.30	0.29
	assign (segid 3A4 and resid 307 and name CA) (segid 3A4 and resid 316 and name CA)	14.13	0.12	0.12
	assign (segid 3A4 and resid 307 and name CA) (segid 3A4 and resid 317 and name CA)	15.07	0.41	0.42
	assign (segid 3A4 and resid 307 and name CA) (segid 3A4 and resid 318 and name CA)	17.32	0.55	0.54
	assign (segid 3A4 and resid 307 and name CA) (segid 3A4 and resid 318 and name CB)	16.90	0.59	0.58
35	assign (segid 3A4 and resid 307 and name CA) (segid 3A4 and resid 318 and name N)	19.04	0.33	0.32
	assign (segid 3A4 and resid 307 and name CA) (segid 3A4 and resid 347 and name CA)	18.52	0.39	0.39
	assign (segid 3A4 and resid 307 and name CA) (segid 3A4 and resid 347 and name CB)	18.20	0.34	0.35
	assign (segid 3A4 and resid 307 and name CA) (segid 3A4 and resid 348 and name CA)	18.41	0.43	0.42
	assign (segid 3A4 and resid 307 and name CA) (segid 3A4 and resid 350 and name CA)	18.33	0.52	0.52
40	assign (segid 3A4 and resid 307 and name CA) (segid 3A4 and resid 351 and name CA)	14.98	0.30	0.30
	assign (segid 3A4 and resid 307 and name CA) (segid 3A4 and resid 352 and name CA)	16.79	0.40	0.41
	assign (segid 3A4 and resid 307 and name CA) (segid 3A4 and resid 352 and name CB)	17.56	0.37	0.38
	assign (segid 3A4 and resid 307 and name CA) (segid 3A4 and resid 353 and name CA)	18.81	0.61	0.61
	assign (segid 3A4 and resid 307 and name CA) (segid 3A4 and resid 353 and name CB)	19.03	0.71	0.70
45	assign (segid 3A4 and resid 307 and name CA) (segid 3A4 and resid 354 and name CA)	19.33	0.64	0.64
	assign (segid 3A4 and resid 307 and name CA) (segid 3A4 and resid 356 and name CA)	16.85	0.83	0.83
	assign (segid 3A4 and resid 307 and name CA) (segid 3A4 and resid 356 and name CB)	16.58	0.76	0.76
	assign (segid 3A4 and resid 307 and name CA) (segid 3A4 and resid 357 and name CA)	14.55	0.68	0.69
	assign (segid 3A4 and resid 307 and name CA) (segid 3A4 and resid 357 and name CB)	13.78	0.67	0.67
50	assign (segid 3A4 and resid 307 and name CA) (segid 3A4 and resid 358 and name CA)	16.66	1.03	1.02
	assign (segid 3A4 and resid 307 and name CA) (segid 3A4 and resid 359 and name CA)	16.64	0.39	0.39
	assign (segid 3A4 and resid 307 and name CA) (segid 3A4 and resid 359 and name CB)	16.38	0.32	0.33
	assign (segid 3A4 and resid 307 and name CA) (segid 3A4 and resid 360 and name CA)	15.34	0.33	0.32
	assign (segid 3A4 and resid 307 and name CA) (segid 3A4 and resid 360 and name CB)	16.28	0.34	0.34
55	assign (segid 3A4 and resid 307 and name CA) (segid 3A4 and resid 361 and name CA)	16.41	0.21	0.21
	assign (segid 3A4 and resid 307 and name CA) (segid 3A4 and resid 361 and name CB)	17.88	0.21	0.21
	assign (segid 3A4 and resid 307 and name CA) (segid 3A4 and resid 362 and name CA)	14.33	0.23	0.23
	assign (segid 3A4 and resid 307 and name CA) (segid 3A4 and resid 362 and name CB)	14.56	0.30	0.29
	assign (segid 3A4 and resid 307 and name CA) (segid 3A4 and resid 363 and name CA)	11.23	0.22	0.23
60	assign (segid 3A4 and resid 307 and name CA) (segid 3A4 and resid 363 and name CB)	11.46	0.26	0.27
	assign (segid 3A4 and resid 307 and name CA) (segid 3A4 and resid 364 and name CA)	9.15	0.19	0.20
	assign (segid 3A4 and resid 307 and name CA) (segid 3A4 and resid 364 and name CB)	10.04	0.16	0.15
	assign (segid 3A4 and resid 307 and name CA) (segid 3A4 and resid 364 and name O)	7.30	0.11	0.11
	assign (segid 3A4 and resid 307 and name CA) (segid 3A4 and resid 365 and name C)	5.44	0.22	0.22
65	assign (segid 3A4 and resid 307 and name CA) (segid 3A4 and resid 365 and name CA)	5.62	0.32	0.33
	assign (segid 3A4 and resid 307 and name CA) (segid 3A4 and resid 365 and name CB)	5.49	0.48	0.49
	assign (segid 3A4 and resid 307 and name CA) (segid 3A4 and resid 365 and name N)	7.02	0.31	0.30
	assign (segid 3A4 and resid 307 and name CA) (segid 3A4 and resid 365 and name O)	4.48	0.17	0.18
	assign (segid 3A4 and resid 307 and name CA) (segid 3A4 and resid 381 and name CA)	12.34	0.41	0.41
70	assign (segid 3A4 and resid 307 and name CA) (segid 3A4 and resid 382 and name CA)	15.03	0.19	0.20
	assign (segid 3A4 and resid 307 and name CA) (segid 3A4 and resid 382 and name CB)	16.43	0.24	0.24
	assign (segid 3A4 and resid 307 and name CA) (segid 3A4 and resid 383 and name CA)	14.09	0.25	0.25
	assign (segid 3A4 and resid 307 and name CA) (segid 3A4 and resid 384 and name CA)	15.46	0.52	0.53
	assign (segid 3A4 and resid 307 and name CA) (segid 3A4 and resid 384 and name CB)	14.77	0.63	0.64
75	assign (segid 3A4 and resid 307 and name CA) (segid 3A4 and resid 385 and name CA)	18.32	0.42	0.43
	assign (segid 3A4 and resid 307 and name CA) (segid 3A4 and resid 391 and name CB)	17.72	0.72	0.71
	assign (segid 3A4 and resid 307 and name CA) (segid 3A4 and resid 394 and name CA)	14.93	0.79	0.79
	assign (segid 3A4 and resid 307 and name CA) (segid 3A4 and resid 394 and name CB)	14.73	0.86	0.86
	assign (segid 3A4 and resid 307 and name CA) (segid 3A4 and resid 395 and name CA)	14.55	0.86	0.86
80	assign (segid 3A4 and resid 307 and name CA) (segid 3A4 and resid 396 and name CA)	15.16	0.68	0.67
	assign (segid 3A4 and resid 307 and name CA) (segid 3A4 and resid 396 and name CB)	17.59	0.68	0.69
	assign (segid 3A4 and resid 307 and name CA) (segid 3A4 and resid 397 and name CA)	14.20	0.71	0.71
	assign (segid 3A4 and resid 307 and name CA) (segid 3A4 and resid 397 and name CB)	14.22	0.74	0.74

	assign (segid 3A4 and resid 307 and name CA)	(segid 3A4 and resid 398 and name CA)	10.77	0.71	0.71
	assign (segid 3A4 and resid 307 and name CA)	(segid 3A4 and resid 398 and name CB)	10.20	0.80	0.80
	assign (segid 3A4 and resid 307 and name CA)	(segid 3A4 and resid 399 and name CA)	12.63	0.61	0.61
	assign (segid 3A4 and resid 307 and name CA)	(segid 3A4 and resid 399 and name CB)	13.92	0.63	0.64
5	assign (segid 3A4 and resid 307 and name CA)	(segid 3A4 and resid 400 and name CA)	14.28	0.56	0.56
	assign (segid 3A4 and resid 307 and name CA)	(segid 3A4 and resid 400 and name CB)	15.24	0.52	0.51
	assign (segid 3A4 and resid 307 and name CA)	(segid 3A4 and resid 401 and name CA)	11.40	0.45	0.45
	assign (segid 3A4 and resid 307 and name CA)	(segid 3A4 and resid 402 and name CA)	9.66	0.51	0.51
	assign (segid 3A4 and resid 307 and name CA)	(segid 3A4 and resid 402 and name CB)	9.24	0.50	0.50
10	assign (segid 3A4 and resid 307 and name CA)	(segid 3A4 and resid 403 and name CA)	13.23	0.51	0.52
	assign (segid 3A4 and resid 307 and name CA)	(segid 3A4 and resid 403 and name CB)	14.39	0.51	0.51
	assign (segid 3A4 and resid 307 and name CA)	(segid 3A4 and resid 404 and name CA)	14.33	0.65	0.65
	assign (segid 3A4 and resid 307 and name CA)	(segid 3A4 and resid 404 and name CB)	14.53	0.70	0.70
	assign (segid 3A4 and resid 307 and name CA)	(segid 3A4 and resid 405 and name CA)	11.82	0.67	0.67
	assign (segid 3A4 and resid 307 and name CA)	(segid 3A4 and resid 405 and name CB)	10.46	0.62	0.62
15	assign (segid 3A4 and resid 307 and name CA)	(segid 3A4 and resid 406 and name CA)	12.18	0.53	0.53
	assign (segid 3A4 and resid 307 and name CA)	(segid 3A4 and resid 407 and name CA)	15.88	0.52	0.52
	assign (segid 3A4 and resid 307 and name CA)	(segid 3A4 and resid 407 and name CB)	16.67	0.55	0.55
	assign (segid 3A4 and resid 307 and name CA)	(segid 3A4 and resid 408 and name CA)	16.48	0.59	0.59
	assign (segid 3A4 and resid 307 and name CA)	(segid 3A4 and resid 408 and name CB)	16.02	0.67	0.67
20	assign (segid 3A4 and resid 307 and name CA)	(segid 3A4 and resid 409 and name CA)	15.26	0.63	0.63
	assign (segid 3A4 and resid 307 and name CA)	(segid 3A4 and resid 409 and name CB)	13.95	0.72	0.71
	assign (segid 3A4 and resid 307 and name CA)	(segid 3A4 and resid 410 and name CA)	17.08	0.37	0.36
	assign (segid 3A4 and resid 307 and name CB)	(segid 3A4 and resid 308 and name C)	5.42	0.03	0.02
25	assign (segid 3A4 and resid 307 and name CB)	(segid 3A4 and resid 308 and name CA)	4.48	0.05	0.06
	assign (segid 3A4 and resid 307 and name CB)	(segid 3A4 and resid 308 and name CB)	5.36	0.11	0.10
	assign (segid 3A4 and resid 307 and name CB)	(segid 3A4 and resid 308 and name N)	3.15	0.07	0.08
	assign (segid 3A4 and resid 307 and name CB)	(segid 3A4 and resid 308 and name O)	6.25	0.05	0.04
	assign (segid 3A4 and resid 307 and name CB)	(segid 3A4 and resid 309 and name C)	6.86	0.08	0.09
30	assign (segid 3A4 and resid 307 and name CB)	(segid 3A4 and resid 309 and name CA)	6.82	0.10	0.10
	assign (segid 3A4 and resid 307 and name CB)	(segid 3A4 and resid 309 and name CB)	7.31	0.18	0.17
	assign (segid 3A4 and resid 307 and name CB)	(segid 3A4 and resid 309 and name N)	5.63	0.10	0.10
	assign (segid 3A4 and resid 307 and name CB)	(segid 3A4 and resid 310 and name C)	6.81	0.15	0.15
	assign (segid 3A4 and resid 307 and name CB)	(segid 3A4 and resid 310 and name CA)	6.40	0.15	0.15
35	assign (segid 3A4 and resid 307 and name CB)	(segid 3A4 and resid 310 and name CB)	5.66	0.23	0.24
	assign (segid 3A4 and resid 307 and name CB)	(segid 3A4 and resid 310 and name N)	5.94	0.11	0.10
	assign (segid 3A4 and resid 307 and name CB)	(segid 3A4 and resid 311 and name CA)	6.94	0.12	0.12
	assign (segid 3A4 and resid 307 and name CB)	(segid 3A4 and resid 311 and name CB)	6.32	0.11	0.10
	assign (segid 3A4 and resid 307 and name CB)	(segid 3A4 and resid 311 and name CG)	7.50	0.14	0.13
40	assign (segid 3A4 and resid 307 and name CB)	(segid 3A4 and resid 311 and name N)	6.13	0.12	0.12
	assign (segid 3A4 and resid 307 and name CB)	(segid 3A4 and resid 312 and name CA)	9.60	0.06	0.05
	assign (segid 3A4 and resid 307 and name CB)	(segid 3A4 and resid 312 and name CB)	9.72	0.09	0.10
	assign (segid 3A4 and resid 307 and name CB)	(segid 3A4 and resid 313 and name CA)	11.22	0.15	0.15
	assign (segid 3A4 and resid 307 and name CB)	(segid 3A4 and resid 313 and name CB)	10.96	0.23	0.22
45	assign (segid 3A4 and resid 307 and name CB)	(segid 3A4 and resid 314 and name CA)	11.44	0.19	0.20
	assign (segid 3A4 and resid 307 and name CB)	(segid 3A4 and resid 314 and name CB)	10.56	0.23	0.22
	assign (segid 3A4 and resid 307 and name CB)	(segid 3A4 and resid 315 and name CA)	12.87	0.24	0.24
	assign (segid 3A4 and resid 307 and name CB)	(segid 3A4 and resid 315 and name CB)	12.28	0.31	0.31
	assign (segid 3A4 and resid 307 and name CB)	(segid 3A4 and resid 316 and name CA)	15.10	0.10	0.10
50	assign (segid 3A4 and resid 307 and name CB)	(segid 3A4 and resid 317 and name CA)	16.20	0.39	0.38
	assign (segid 3A4 and resid 307 and name CB)	(segid 3A4 and resid 318 and name CA)	18.57	0.53	0.52
	assign (segid 3A4 and resid 307 and name CB)	(segid 3A4 and resid 318 and name CB)	18.20	0.57	0.57
	assign (segid 3A4 and resid 307 and name CB)	(segid 3A4 and resid 348 and name CA)	19.11	0.36	0.36
	assign (segid 3A4 and resid 307 and name CB)	(segid 3A4 and resid 350 and name CA)	19.08	0.43	0.43
55	assign (segid 3A4 and resid 307 and name CB)	(segid 3A4 and resid 350 and name CB)	19.07	0.51	0.51
	assign (segid 3A4 and resid 307 and name CB)	(segid 3A4 and resid 351 and name CA)	15.64	0.31	0.31
	assign (segid 3A4 and resid 307 and name CB)	(segid 3A4 and resid 352 and name CA)	17.23	0.42	0.41
	assign (segid 3A4 and resid 307 and name CB)	(segid 3A4 and resid 352 and name CB)	18.04	0.40	0.39
	assign (segid 3A4 and resid 307 and name CB)	(segid 3A4 and resid 353 and name CA)	19.11	0.63	0.63
60	assign (segid 3A4 and resid 307 and name CB)	(segid 3A4 and resid 353 and name CB)	19.36	0.72	0.73
	assign (segid 3A4 and resid 307 and name CB)	(segid 3A4 and resid 354 and name CA)	19.34	0.68	0.67
	assign (segid 3A4 and resid 307 and name CB)	(segid 3A4 and resid 354 and name CB)	16.89	0.86	0.86
	assign (segid 3A4 and resid 307 and name CB)	(segid 3A4 and resid 356 and name CA)	16.75	0.77	0.78
	assign (segid 3A4 and resid 307 and name CB)	(segid 3A4 and resid 356 and name CB)	14.49	0.72	0.71
65	assign (segid 3A4 and resid 307 and name CB)	(segid 3A4 and resid 357 and name CA)	13.83	0.68	0.68
	assign (segid 3A4 and resid 307 and name CB)	(segid 3A4 and resid 358 and name CA)	16.32	1.05	1.04
	assign (segid 3A4 and resid 307 and name CB)	(segid 3A4 and resid 359 and name CA)	16.34	0.40	0.41
	assign (segid 3A4 and resid 307 and name CB)	(segid 3A4 and resid 359 and name CB)	15.98	0.33	0.34
	assign (segid 3A4 and resid 307 and name CB)	(segid 3A4 and resid 360 and name CA)	15.38	0.34	0.35
	assign (segid 3A4 and resid 307 and name CB)	(segid 3A4 and resid 360 and name CB)	16.39	0.35	0.36
70	assign (segid 3A4 and resid 307 and name CB)	(segid 3A4 and resid 361 and name CA)	16.53	0.23	0.22
	assign (segid 3A4 and resid 307 and name CB)	(segid 3A4 and resid 361 and name CB)	17.99	0.22	0.23
	assign (segid 3A4 and resid 307 and name CB)	(segid 3A4 and resid 362 and name CA)	14.20	0.25	0.25
	assign (segid 3A4 and resid 307 and name CB)	(segid 3A4 and resid 362 and name CB)	14.28	0.32	0.32
75	assign (segid 3A4 and resid 307 and name CB)	(segid 3A4 and resid 363 and name CA)	11.23	0.27	0.27
	assign (segid 3A4 and resid 307 and name CB)	(segid 3A4 and resid 363 and name CB)	11.55	0.31	0.32
	assign (segid 3A4 and resid 307 and name CB)	(segid 3A4 and resid 364 and name C)	7.23	0.20	0.21
	assign (segid 3A4 and resid 307 and name CB)	(segid 3A4 and resid 364 and name CA)	8.71	0.22	0.23
	assign (segid 3A4 and resid 307 and name CB)	(segid 3A4 and resid 364 and name CB)	9.47	0.17	0.18
80	assign (segid 3A4 and resid 307 and name CB)	(segid 3A4 and resid 364 and name O)	6.88	0.09	0.09
	assign (segid 3A4 and resid 307 and name CB)	(segid 3A4 and resid 365 and name C)	4.61	0.22	0.23
	assign (segid 3A4 and resid 307 and name CB)	(segid 3A4 and resid 365 and name CA)	5.10	0.37	0.37
	assign (segid 3A4 and resid 307 and name CB)	(segid 3A4 and resid 365 and name CB)	4.97	0.58	0.59

	assign	(segid 3A4 and resid 307 and name CB)	(segid 3A4 and resid 365 and name N)	6.52	0.35	0.36
	assign	(segid 3A4 and resid 307 and name CB)	(segid 3A4 and resid 365 and name O)	3.60	0.17	0.17
	assign	(segid 3A4 and resid 307 and name CB)	(segid 3A4 and resid 381 and name CA)	13.15	0.43	0.41
	assign	(segid 3A4 and resid 307 and name CB)	(segid 3A4 and resid 382 and name CA)	16.05	0.26	0.27
5	assign	(segid 3A4 and resid 307 and name CB)	(segid 3A4 and resid 382 and name CB)	17.40	0.29	0.30
	assign	(segid 3A4 and resid 307 and name CB)	(segid 3A4 and resid 383 and name CA)	15.31	0.30	0.30
	assign	(segid 3A4 and resid 307 and name CB)	(segid 3A4 and resid 384 and name CA)	16.79	0.60	0.60
	assign	(segid 3A4 and resid 307 and name CB)	(segid 3A4 and resid 384 and name CB)	16.11	0.72	0.71
	assign	(segid 3A4 and resid 307 and name CB)	(segid 3A4 and resid 385 and name CA)	19.52	0.51	0.52
10	assign	(segid 3A4 and resid 307 and name CB)	(segid 3A4 and resid 394 and name CA)	16.36	0.84	0.83
	assign	(segid 3A4 and resid 307 and name CB)	(segid 3A4 and resid 394 and name CB)	16.11	0.90	0.91
	assign	(segid 3A4 and resid 307 and name CB)	(segid 3A4 and resid 395 and name CA)	15.89	0.90	0.91
	assign	(segid 3A4 and resid 307 and name CB)	(segid 3A4 and resid 396 and name CA)	17.56	0.70	0.70
	assign	(segid 3A4 and resid 307 and name CB)	(segid 3A4 and resid 397 and name CA)	15.69	0.72	0.71
15	assign	(segid 3A4 and resid 307 and name CB)	(segid 3A4 and resid 397 and name CB)	15.72	0.75	0.75
	assign	(segid 3A4 and resid 307 and name CB)	(segid 3A4 and resid 398 and name CA)	12.21	0.72	0.73
	assign	(segid 3A4 and resid 307 and name CB)	(segid 3A4 and resid 398 and name CB)	11.62	0.82	0.82
	assign	(segid 3A4 and resid 307 and name CB)	(segid 3A4 and resid 399 and name CA)	13.91	0.64	0.64
20	assign	(segid 3A4 and resid 307 and name CB)	(segid 3A4 and resid 399 and name CB)	15.19	0.67	0.66
	assign	(segid 3A4 and resid 307 and name CB)	(segid 3A4 and resid 400 and name CA)	15.61	0.57	0.56
	assign	(segid 3A4 and resid 307 and name CB)	(segid 3A4 and resid 400 and name CB)	16.61	0.52	0.52
	assign	(segid 3A4 and resid 307 and name CB)	(segid 3A4 and resid 401 and name CA)	12.74	0.45	0.44
	assign	(segid 3A4 and resid 307 and name CB)	(segid 3A4 and resid 402 and name CA)	10.79	0.55	0.54
25	assign	(segid 3A4 and resid 307 and name CB)	(segid 3A4 and resid 402 and name CB)	10.36	0.54	0.53
	assign	(segid 3A4 and resid 307 and name CB)	(segid 3A4 and resid 403 and name CA)	14.23	0.56	0.56
	assign	(segid 3A4 and resid 307 and name CB)	(segid 3A4 and resid 403 and name CB)	15.43	0.55	0.55
	assign	(segid 3A4 and resid 307 and name CB)	(segid 3A4 and resid 404 and name CA)	15.35	0.69	0.70
	assign	(segid 3A4 and resid 307 and name CB)	(segid 3A4 and resid 404 and name CB)	15.64	0.74	0.74
30	assign	(segid 3A4 and resid 307 and name CB)	(segid 3A4 and resid 405 and name CA)	12.66	0.76	0.76
	assign	(segid 3A4 and resid 307 and name CB)	(segid 3A4 and resid 405 and name CB)	11.33	0.71	0.71
	assign	(segid 3A4 and resid 307 and name CB)	(segid 3A4 and resid 406 and name CA)	12.75	0.61	0.62
	assign	(segid 3A4 and resid 307 and name CB)	(segid 3A4 and resid 407 and name CA)	16.50	0.62	0.62
	assign	(segid 3A4 and resid 307 and name CB)	(segid 3A4 and resid 407 and name CB)	17.38	0.63	0.62
35	assign	(segid 3A4 and resid 307 and name CB)	(segid 3A4 and resid 408 and name CA)	17.09	0.70	0.71
	assign	(segid 3A4 and resid 307 and name CB)	(segid 3A4 and resid 408 and name CB)	16.70	0.76	0.76
	assign	(segid 3A4 and resid 307 and name CB)	(segid 3A4 and resid 409 and name CA)	15.57	0.75	0.76
	assign	(segid 3A4 and resid 307 and name CB)	(segid 3A4 and resid 409 and name CB)	14.21	0.83	0.82
	assign	(segid 3A4 and resid 307 and name CB)	(segid 3A4 and resid 410 and name CA)	17.27	0.47	0.47
40	assign	(segid 3A4 and resid 307 and name N)	(segid 3A4 and resid 307 and name C)	2.43	0.02	0.02
	assign	(segid 3A4 and resid 307 and name N)	(segid 3A4 and resid 307 and name CA)	1.45	0.01	0.01
	assign	(segid 3A4 and resid 307 and name N)	(segid 3A4 and resid 307 and name CB)	2.44	0.01	0.01
	assign	(segid 3A4 and resid 307 and name N)	(segid 3A4 and resid 307 and name O)	3.50	0.03	0.04
	assign	(segid 3A4 and resid 307 and name N)	(segid 3A4 and resid 308 and name C)	4.64	0.03	0.03
45	assign	(segid 3A4 and resid 307 and name N)	(segid 3A4 and resid 308 and name CA)	4.16	0.03	0.02
	assign	(segid 3A4 and resid 307 and name N)	(segid 3A4 and resid 308 and name CB)	4.89	0.05	0.05
	assign	(segid 3A4 and resid 307 and name N)	(segid 3A4 and resid 308 and name N)	2.76	0.04	0.04
	assign	(segid 3A4 and resid 307 and name N)	(segid 3A4 and resid 308 and name O)	5.70	0.06	0.05
	assign	(segid 3A4 and resid 307 and name N)	(segid 3A4 and resid 309 and name C)	5.58	0.05	0.06
50	assign	(segid 3A4 and resid 307 and name N)	(segid 3A4 and resid 3			

	assign	(segid 3A4 and resid 307 and name O)	(segid 3A4 and resid 311 and name CD)	5.85	0.12	0.12
	assign	(segid 3A4 and resid 307 and name O)	(segid 3A4 and resid 311 and name CG)	4.94	0.08	0.08
	assign	(segid 3A4 and resid 307 and name O)	(segid 3A4 and resid 311 and name N)	2.98	0.13	0.13
	assign	(segid 3A4 and resid 307 and name O)	(segid 3A4 and resid 311 and name O)	6.13	0.09	0.09
5	assign	(segid 3A4 and resid 307 and name O)	(segid 3A4 and resid 311 and name OE1)	5.71	0.16	0.16
	assign	(segid 3A4 and resid 307 and name O)	(segid 3A4 and resid 312 and name C)	7.29	0.05	0.05
	assign	(segid 3A4 and resid 307 and name O)	(segid 3A4 and resid 312 and name CA)	6.41	0.05	0.06
	assign	(segid 3A4 and resid 307 and name O)	(segid 3A4 and resid 312 and name CB)	6.69	0.08	0.08
	assign	(segid 3A4 and resid 307 and name O)	(segid 3A4 and resid 312 and name N)	5.05	0.05	0.06
10	assign	(segid 3A4 and resid 307 and name O)	(segid 3A4 and resid 313 and name N)	6.99	0.11	0.11
	assign	(segid 3A4 and resid 307 and name O)	(segid 3A4 and resid 314 and name CB)	7.74	0.14	0.14
	assign	(segid 3A4 and resid 307 and name O)	(segid 3A4 and resid 364 and name C)	6.18	0.16	0.15
	assign	(segid 3A4 and resid 307 and name O)	(segid 3A4 and resid 364 and name CA)	7.57	0.15	0.14
	assign	(segid 3A4 and resid 307 and name O)	(segid 3A4 and resid 364 and name N)	7.76	0.14	0.13
15	assign	(segid 3A4 and resid 307 and name O)	(segid 3A4 and resid 364 and name O)	5.79	0.15	0.16
	assign	(segid 3A4 and resid 307 and name O)	(segid 3A4 and resid 365 and name C)	4.80	0.25	0.25
	assign	(segid 3A4 and resid 307 and name O)	(segid 3A4 and resid 365 and name CA)	4.50	0.31	0.30
	assign	(segid 3A4 and resid 307 and name O)	(segid 3A4 and resid 365 and name CB)	4.66	0.42	0.43
	assign	(segid 3A4 and resid 307 and name O)	(segid 3A4 and resid 365 and name N)	5.67	0.26	0.27
20	assign	(segid 3A4 and resid 307 and name O)	(segid 3A4 and resid 365 and name O)	4.19	0.26	0.26
	assign	(segid 3A4 and resid 308 and name C)	(segid 3A4 and resid 308 and name CB)	2.53	0.03	0.03
	assign	(segid 3A4 and resid 308 and name C)	(segid 3A4 and resid 308 and name O)	1.23	0.00	0.01
	assign	(segid 3A4 and resid 308 and name C)	(segid 3A4 and resid 309 and name C)	3.00	0.06	0.06
	assign	(segid 3A4 and resid 308 and name C)	(segid 3A4 and resid 309 and name CA)	2.45	0.02	0.02
25	assign	(segid 3A4 and resid 308 and name C)	(segid 3A4 and resid 309 and name CB)	3.75	0.02	0.02
	assign	(segid 3A4 and resid 308 and name C)	(segid 3A4 and resid 309 and name N)	1.34	0.01	0.00
	assign	(segid 3A4 and resid 308 and name C)	(segid 3A4 and resid 309 and name O)	3.82	0.05	0.06
	assign	(segid 3A4 and resid 308 and name C)	(segid 3A4 and resid 310 and name C)	4.51	0.12	0.12
	assign	(segid 3A4 and resid 308 and name C)	(segid 3A4 and resid 310 and name CA)	4.44	0.12	0.11
30	assign	(segid 3A4 and resid 308 and name C)	(segid 3A4 and resid 310 and name CB)	5.18	0.13	0.13
	assign	(segid 3A4 and resid 308 and name C)	(segid 3A4 and resid 310 and name N)	3.27	0.11	0.12
	assign	(segid 3A4 and resid 308 and name C)	(segid 3A4 and resid 310 and name O)	5.57	0.13	0.12
	assign	(segid 3A4 and resid 308 and name C)	(segid 3A4 and resid 311 and name C)	4.75	0.05	0.06
	assign	(segid 3A4 and resid 308 and name C)	(segid 3A4 and resid 311 and name CA)	4.50	0.10	0.09
35	assign	(segid 3A4 and resid 308 and name C)	(segid 3A4 and resid 311 and name CB)	4.38	0.08	0.09
	assign	(segid 3A4 and resid 308 and name C)	(segid 3A4 and resid 311 and name CD)	6.92	0.08	0.09
	assign	(segid 3A4 and resid 308 and name C)	(segid 3A4 and resid 311 and name CG)	5.59	0.07	0.08
	assign	(segid 3A4 and resid 308 and name C)	(segid 3A4 and resid 311 and name N)	3.77	0.09	0.10
	assign	(segid 3A4 and resid 308 and name C)	(segid 3A4 and resid 311 and name O)	5.96	0.06	0.05
40	assign	(segid 3A4 and resid 308 and name C)	(segid 3A4 and resid 311 and name OE1)	7.14	0.11	0.11
	assign	(segid 3A4 and resid 308 and name C)	(segid 3A4 and resid 312 and name C)	6.07	0.06	0.05
	assign	(segid 3A4 and resid 308 and name C)	(segid 3A4 and resid 312 and name CA)	4.94	0.07	0.08
	assign	(segid 3A4 and resid 308 and name C)	(segid 3A4 and resid 312 and name CB)	4.58	0.13	0.13
	assign	(segid 3A4 and resid 308 and name C)	(segid 3A4 and resid 312 and name N)	4.03	0.04	0.05
45	assign	(segid 3A4 and resid 308 and name C)	(segid 3A4 and resid 312 and name O)	7.21	0.07	0.07
	assign	(segid 3A4 and resid 308 and name C)	(segid 3A4 and resid 313 and name CA)	7.30	0.06	0.05
	assign	(segid 3A4 and resid 308 and name C)	(segid 3A4 and resid 313 and name CB)	7.38	0.09	0.10
	assign	(segid 3A4 and resid 308 and name C)	(segid 3A4 and resid 313 and name CG)	7.21	0.15	0.16
	assign	(segid 3A4 and resid 308 and name C)	(segid 3A4 and resid 313 and name N)	5.98	0.06	0.06
50	assign	(segid 3A4 and resid 308 and name C)	(segid 3A4 and resid 314 and name N)	7.71	0.05	0.04
	assign	(segid 3A4 and resid 308 and name C)	(segid 3A4 and resid 363 and name CG)	7.54	0.28	0.29
	assign	(segid 3A4 and resid 308 and name C)	(segid 3A4 and resid 364 and name C)	7.45	0.12	0.11
	assign	(segid 3A4 and resid 308 and name C)	(segid 3A4 and resid 365 and name C)	6.70	0.23	0.22
	assign	(segid 3A4 and resid 308 and name C)	(segid 3A4 and resid 365 and name CA)	5.82	0.13	0.13
55	assign	(segid 3A4 and resid 308 and name C)	(segid 3A4 and resid 365 and name CB)	5.41	0.16	0.15
	assign	(segid 3A4 and resid 308 and name C)	(segid 3A4 and resid 365 and name N)	6.73	0.08	0.08
	assign	(segid 3A4 and resid 308 and name C)	(segid 3A4 and resid 365 and name O)	6.43	0.34	0.34
	assign	(segid 3A4 and resid 308 and name CA)	(segid 3A4 and resid 308 and name C)	1.53	0.00	0.01
	assign	(segid 3A4 and resid 308 and name CA)	(segid 3A4 and resid 308 and name CB)	1.55	0.02	0.02
60	assign	(segid 3A4 and resid 308 and name CA)	(segid 3A4 and resid 308 and name O)	2.40	0.01	0.01
	assign	(segid 3A4 and resid 308 and name CA)	(segid 3A4 and resid 309 and name C)	4.41	0.06	0.05
	assign	(segid 3A4 and resid 308 and name CA)	(segid 3A4 and resid 309 and name CA)	3.83	0.02	0.03
	assign	(segid 3A4 and resid 308 and name CA)	(segid 3A4 and resid 309 and name CB)	4.92	0.04	0.03
	assign	(segid 3A4 and resid 308 and name CA)	(segid 3A4 and resid 309 and name N)	2.45	0.02	0.02
65	assign	(segid 3A4 and resid 308 and name CA)	(segid 3A4 and resid 309 and name O)	5.29	0.04	0.05
	assign	(segid 3A4 and resid 308 and name CA)	(segid 3A4 and resid 310 and name C)	5.47	0.13	0.13
	assign	(segid 3A4 and resid 308 and name CA)	(segid 3A4 and resid 310 and name CA)	5.43	0.12	0.13
	assign	(segid 3A4 and resid 308 and name CA)	(segid 3A4 and resid 310 and name CB)	5.84	0.15	0.16
	assign	(segid 3A4 and resid 308 and name CA)	(segid 3A4 and resid 310 and name N)	4.38	0.12	0.12
70	assign	(segid 3A4 and resid 308 and name CA)	(segid 3A4 and resid 310 and name O)	6.59	0.14	0.13
	assign	(segid 3A4 and resid 308 and name CA)	(segid 3A4 and resid 311 and name C)	5.59	0.09	0.10
	assign	(segid 3A4 and resid 308 and name CA)	(segid 3A4 and resid 311 and name CA)	5.09	0.13	0.14
	assign	(segid 3A4 and resid 308 and name CA)	(segid 3A4 and resid 311 and name CB)	4.52	0.13	0.14
	assign	(segid 3A4 and resid 308 and name CA)	(segid 3A4 and resid 311 and name CD)	6.98	0.14	0.14
75	assign	(segid 3A4 and resid 308 and name CA)	(segid 3A4 and resid 311 and name CG)	5.63	0.12	0.12
	assign	(segid 3A4 and resid 308 and name CA)	(segid 3A4 and resid 311 and name N)	4.52	0.13	0.13
	assign	(segid 3A4 and resid 308 and name CA)	(segid 3A4 and resid 311 and name O)	6.76	0.10	0.10
	assign	(segid 3A4 and resid 308 and name CA)	(segid 3A4 and resid 311 and name OE1)	7.28	0.16	0.16
	assign	(segid 3A4 and resid 308 and name CA)	(segid 3A4 and resid 312 and name C)	7.33	0.06	0.06
80	assign	(segid 3A4 and resid 308 and name CA)	(segid 3A4 and resid 312 and name CA)	6.10	0.08	0.07
	assign	(segid 3A4 and resid 308 and name CA)	(segid 3A4 and resid 312 and name CB)	5.83	0.11	0.11
	assign	(segid 3A4 and resid 308 and name CA)	(segid 3A4 and resid 312 and name N)	5.10	0.05	0.06
	assign	(segid 3A4 and resid 308 and name CA)	(segid 3A4 and resid 313 and name CA)	8.68	0.06	0.05

5	assign	(segid 3A4 and resid 308 and name CA)	(segid 3A4 and resid 313 and name CB)	8.79	0.10	0.10
	assign	(segid 3A4 and resid 308 and name CA)	(segid 3A4 and resid 313 and name N)	7.34	0.06	0.06
	assign	(segid 3A4 and resid 308 and name CA)	(segid 3A4 and resid 314 and name CA)	9.78	0.09	0.09
	assign	(segid 3A4 and resid 308 and name CA)	(segid 3A4 and resid 314 and name CB)	9.35	0.10	0.09
	assign	(segid 3A4 and resid 308 and name CA)	(segid 3A4 and resid 315 and name CA)	10.35	0.23	0.22
10	assign	(segid 3A4 and resid 308 and name CA)	(segid 3A4 and resid 315 and name CB)	9.53	0.30	0.30
	assign	(segid 3A4 and resid 308 and name CA)	(segid 3A4 and resid 316 and name CA)	11.92	0.22	0.22
	assign	(segid 3A4 and resid 308 and name CA)	(segid 3A4 and resid 317 and name CA)	13.62	0.30	0.30
	assign	(segid 3A4 and resid 308 and name CA)	(segid 3A4 and resid 318 and name CA)	15.55	0.50	0.50
	assign	(segid 3A4 and resid 308 and name CA)	(segid 3A4 and resid 318 and name CB)	15.06	0.52	0.53
15	assign	(segid 3A4 and resid 308 and name CA)	(segid 3A4 and resid 319 and name CA)	18.35	0.44	0.44
	assign	(segid 3A4 and resid 308 and name CA)	(segid 3A4 and resid 319 and name CB)	18.43	0.39	0.38
	assign	(segid 3A4 and resid 308 and name CA)	(segid 3A4 and resid 347 and name CA)	18.73	0.32	0.32
	assign	(segid 3A4 and resid 308 and name CA)	(segid 3A4 and resid 347 and name CB)	18.21	0.39	0.38
	assign	(segid 3A4 and resid 308 and name CA)	(segid 3A4 and resid 348 and name CA)	17.29	0.37	0.38
20	assign	(segid 3A4 and resid 308 and name CA)	(segid 3A4 and resid 350 and name CA)	18.49	0.31	0.30
	assign	(segid 3A4 and resid 308 and name CA)	(segid 3A4 and resid 350 and name CB)	18.58	0.41	0.42
	assign	(segid 3A4 and resid 308 and name CA)	(segid 3A4 and resid 351 and name CA)	14.85	0.25	0.24
	assign	(segid 3A4 and resid 308 and name CA)	(segid 3A4 and resid 352 and name CA)	16.25	0.34	0.33
	assign	(segid 3A4 and resid 308 and name CA)	(segid 3A4 and resid 352 and name CB)	16.72	0.31	0.31
25	assign	(segid 3A4 and resid 308 and name CA)	(segid 3A4 and resid 353 and name CA)	18.89	0.47	0.46
	assign	(segid 3A4 and resid 308 and name CA)	(segid 3A4 and resid 353 and name CB)	19.34	0.52	0.51
	assign	(segid 3A4 and resid 308 and name CA)	(segid 3A4 and resid 356 and name CA)	17.96	0.68	0.69
	assign	(segid 3A4 and resid 308 and name CA)	(segid 3A4 and resid 356 and name CB)	17.67	0.64	0.63
	assign	(segid 3A4 and resid 308 and name CA)	(segid 3A4 and resid 357 and name CA)	15.19	0.59	0.60
30	assign	(segid 3A4 and resid 308 and name CA)	(segid 3A4 and resid 357 and name CB)	14.18	0.61	0.62
	assign	(segid 3A4 and resid 308 and name CA)	(segid 3A4 and resid 358 and name CA)	16.91	0.83	0.83
	assign	(segid 3A4 and resid 308 and name CA)	(segid 3A4 and resid 359 and name CA)	16.09	0.23	0.24
	assign	(segid 3A4 and resid 308 and name CA)	(segid 3A4 and resid 359 and name CB)	15.78	0.21	0.22
	assign	(segid 3A4 and resid 308 and name CA)	(segid 3A4 and resid 360 and name CA)	14.62	0.19	0.19
35	assign	(segid 3A4 and resid 308 and name CA)	(segid 3A4 and resid 360 and name CB)	15.69	0.24	0.23
	assign	(segid 3A4 and resid 308 and name CA)	(segid 3A4 and resid 361 and name CA)	14.83	0.18	0.17
	assign	(segid 3A4 and resid 308 and name CA)	(segid 3A4 and resid 361 and name CB)	16.21	0.21	0.21
	assign	(segid 3A4 and resid 308 and name CA)	(segid 3A4 and resid 362 and name CA)	12.62	0.14	0.15
	assign	(segid 3A4 and resid 308 and name CA)	(segid 3A4 and resid 362 and name CB)	13.09	0.16	0.16
40	assign	(segid 3A4 and resid 308 and name CA)	(segid 3A4 and resid 363 and name CA)	9.04	0.18	0.18
	assign	(segid 3A4 and resid 308 and name CA)	(segid 3A4 and resid 363 and name CB)	8.83	0.26	0.26
	assign	(segid 3A4 and resid 308 and name CA)	(segid 3A4 and resid 363 and name CG)	7.46	0.30	0.30
	assign	(segid 3A4 and resid 308 and name CA)	(segid 3A4 and resid 364 and name C)	6.68	0.13	0.13
	assign	(segid 3A4 and resid 308 and name CA)	(segid 3A4 and resid 364 and name CA)	7.87	0.09	0.09
45	assign	(segid 3A4 and resid 308 and name CA)	(segid 3A4 and resid 364 and name CB)	9.16	0.10	0.11
	assign	(segid 3A4 and resid 308 and name CA)	(segid 3A4 and resid 364 and name O)	6.80	0.24	0.25
	assign	(segid 3A4 and resid 308 and name CA)	(segid 3A4 and resid 365 and name C)	5.59	0.28	0.28
	assign	(segid 3A4 and resid 308 and name CA)	(segid 3A4 and resid 365 and name CA)	4.77	0.14	0.13
	assign	(segid 3A4 and resid 308 and name CA)	(segid 3A4 and resid 365 and name CB)	4.13	0.13	0.13
50	assign	(segid 3A4 and resid 308 and name CA)	(segid 3A4 and resid 365 and name N)	5.79	0.07	0.07
	assign	(segid 3A4 and resid 308 and name CA)	(segid 3A4 and resid 365 and name O)	5.35	0.44	0.43
	assign	(segid 3A4 and resid 308 and name CA)	(segid 3A4 and resid 381 and name CA)	13.34	0.42	0.42
	assign	(segid 3A4 and resid 308 and name CA)	(segid 3A4 and resid 382 and name CA)	15.70	0.16	0.16
	assign	(segid 3A4 and resid 308 and name CA)	(segid 3A4 and resid 382 and name CB)	17.08	0.23	0.23
55						

	assign (segid 3A4 and resid 308 and name CA) (segid 3A4 and resid 409 and name CB)	11.37	0.59	0.58
	assign (segid 3A4 and resid 308 and name CA) (segid 3A4 and resid 410 and name CA)	15.11	0.31	0.30
	assign (segid 3A4 and resid 308 and name CA) (segid 3A4 and resid 411 and name CA)	17.79	0.46	0.46
	assign (segid 3A4 and resid 308 and name CA) (segid 3A4 and resid 411 and name CB)	18.11	0.61	0.60
	assign (segid 3A4 and resid 308 and name CA) (segid 3A4 and resid 412 and name CA)	17.40	0.61	0.62
5	assign (segid 3A4 and resid 308 and name CA) (segid 3A4 and resid 413 and name CA)	17.84	0.98	0.99
	assign (segid 3A4 and resid 308 and name CA) (segid 3A4 and resid 414 and name CA)	17.05	1.07	1.06
	assign (segid 3A4 and resid 308 and name CA) (segid 3A4 and resid 309 and name C)	5.43	0.07	0.07
	assign (segid 3A4 and resid 308 and name CB) (segid 3A4 and resid 309 and name CB)	4.49	0.06	0.06
	assign (segid 3A4 and resid 308 and name CB) (segid 3A4 and resid 309 and name CA)	5.37	0.06	0.06
10	assign (segid 3A4 and resid 308 and name CB) (segid 3A4 and resid 309 and name N)	3.15	0.04	0.05
	assign (segid 3A4 and resid 308 and name CB) (segid 3A4 and resid 309 and name O)	6.29	0.05	0.05
	assign (segid 3A4 and resid 308 and name CB) (segid 3A4 and resid 310 and name C)	6.90	0.13	0.14
	assign (segid 3A4 and resid 308 and name CB) (segid 3A4 and resid 310 and name CA)	6.82	0.13	0.12
	assign (segid 3A4 and resid 308 and name CB) (segid 3A4 and resid 310 and name CB)	7.29	0.16	0.16
15	assign (segid 3A4 and resid 308 and name CB) (segid 3A4 and resid 310 and name N)	5.63	0.13	0.12
	assign (segid 3A4 and resid 308 and name CB) (segid 3A4 and resid 311 and name C)	6.77	0.10	0.10
	assign (segid 3A4 and resid 308 and name CB) (segid 3A4 and resid 311 and name CA)	6.46	0.14	0.14
	assign (segid 3A4 and resid 308 and name CB) (segid 3A4 and resid 311 and name CB)	5.82	0.16	0.16
	assign (segid 3A4 and resid 308 and name CB) (segid 3A4 and resid 311 and name N)	6.73	0.16	0.15
20	assign (segid 3A4 and resid 308 and name CB) (segid 3A4 and resid 311 and name CA)	5.99	0.14	0.13
	assign (segid 3A4 and resid 308 and name CB) (segid 3A4 and resid 312 and name CA)	6.87	0.10	0.09
	assign (segid 3A4 and resid 308 and name CB) (segid 3A4 and resid 312 and name CB)	6.33	0.13	0.12
	assign (segid 3A4 and resid 308 and name CB) (segid 3A4 and resid 312 and name N)	6.11	0.07	0.07
	assign (segid 3A4 and resid 308 and name CB) (segid 3A4 and resid 313 and name CA)	9.70	0.05	0.05
25	assign (segid 3A4 and resid 308 and name CB) (segid 3A4 and resid 313 and name CB)	9.86	0.09	0.09
	assign (segid 3A4 and resid 308 and name CB) (segid 3A4 and resid 314 and name CA)	11.06	0.08	0.08
	assign (segid 3A4 and resid 308 and name CB) (segid 3A4 and resid 314 and name CB)	10.72	0.10	0.09
	assign (segid 3A4 and resid 308 and name CB) (segid 3A4 and resid 315 and name CA)	11.32	0.24	0.24
	assign (segid 3A4 and resid 308 and name CB) (segid 3A4 and resid 315 and name CB)	10.39	0.31	0.31
30	assign (segid 3A4 and resid 308 and name CB) (segid 3A4 and resid 316 and name CA)	12.65	0.25	0.24
	assign (segid 3A4 and resid 308 and name CB) (segid 3A4 and resid 317 and name CA)	14.56	0.29	0.29
	assign (segid 3A4 and resid 308 and name CB) (segid 3A4 and resid 318 and name CA)	16.25	0.55	0.55
	assign (segid 3A4 and resid 308 and name CB) (segid 3A4 and resid 318 and name CB)	15.68	0.59	0.58
	assign (segid 3A4 and resid 308 and name CB) (segid 3A4 and resid 318 and name N)	18.43	0.39	0.40
35	assign (segid 3A4 and resid 308 and name CB) (segid 3A4 and resid 348 and name CA)	16.21	0.22	0.22
	assign (segid 3A4 and resid 308 and name CB) (segid 3A4 and resid 351 and name CA)	17.50	0.34	0.34
	assign (segid 3A4 and resid 308 and name CB) (segid 3A4 and resid 352 and name CA)	17.89	0.31	0.32
	assign (segid 3A4 and resid 308 and name CB) (segid 3A4 and resid 352 and name CB)	16.56	0.62	0.62
	assign (segid 3A4 and resid 308 and name CB) (segid 3A4 and resid 357 and name CB)	15.55	0.63	0.63
40	assign (segid 3A4 and resid 308 and name CB) (segid 3A4 and resid 357 and name CA)	17.07	0.24	0.25
	assign (segid 3A4 and resid 308 and name CB) (segid 3A4 and resid 359 and name CB)	16.68	0.20	0.20
	assign (segid 3A4 and resid 308 and name CB) (segid 3A4 and resid 359 and name CA)	15.72	0.20	0.21
	assign (segid 3A4 and resid 308 and name CB) (segid 3A4 and resid 360 and name CB)	16.85	0.24	0.24
	assign (segid 3A4 and resid 308 and name CB) (segid 3A4 and resid 361 and name CA)	15.66	0.18	0.18
45	assign (segid 3A4 and resid 308 and name CB) (segid 3A4 and resid 361 and name CB)	17.00	0.22	0.21
	assign (segid 3A4 and resid 308 and name CB) (segid 3A4 and resid 362 and name CA)	13.29	0.17	0.16
	assign (segid 3A4 and resid 308 and name CB) (segid 3A4 and resid 362 and name CB)	13.75	0.17	0.17
	assign (segid 3A4 and resid 308 and name CB) (segid 3A4 and resid 363 and name CA)	9.60	0.19	0.18
	assign (segid 3A4 and resid 308 and name CB) (segid 3A4 and resid 363 and name CB)	9.20	0.26	0.25
50	assign (segid 3A4 and resid 308 and name CB) (segid 3A4 and resid 364 and name C)	7.44	0.22	0.21
	assign (segid 3A4 and resid 308 and name CB) (segid 3A4 and resid 364 and name CA)	8.50	0.16	0.17
	assign (segid 3A4 and resid 308 and name CB) (segid 3A4 and resid 364 and name CB)	9.87	0.19	0.18
	assign (segid 3A4 and resid 308 and name CB) (segid 3A4 and resid 365 and name C)	6.36	0.40	0.40
	assign (segid 3A4 and resid 308 and name CB) (segid 3A4 and resid 365 and name CA)	5.46	0.27	0.28
55	assign (segid 3A4 and resid 308 and name CB) (segid 3A4 and resid 365 and name CB)	4.44	0.21	0.22
	assign (segid 3A4 and resid 308 and name CB) (segid 3A4 and resid 365 and name N)	6.38	0.16	0.16
	assign (segid 3A4 and resid 308 and name CB) (segid 3A4 and resid 365 and name O)	6.24	0.57	0.56
	assign (segid 3A4 and resid 308 and name CB) (segid 3A4 and resid 381 and name CA)	14.83	0.42	0.42
	assign (segid 3A4 and resid 308 and name CB) (segid 3A4 and resid 382 and name CA)	17.09	0.17	0.17
60	assign (segid 3A4 and resid 308 and name CB) (segid 3A4 and resid 382 and name CB)	18.48	0.24	0.24
	assign (segid 3A4 and resid 308 and name CB) (segid 3A4 and resid 383 and name CA)	15.23	0.22	0.22
	assign (segid 3A4 and resid 308 and name CB) (segid 3A4 and resid 384 and name CA)	16.96	0.37	0.37
	assign (segid 3A4 and resid 308 and name CB) (segid 3A4 and resid 384 and name CB)	16.47	0.44	0.45
	assign (segid 3A4 and resid 308 and name CB) (segid 3A4 and resid 394 and name CA)	16.38	0.60	0.60
65	assign (segid 3A4 and resid 308 and name CB) (segid 3A4 and resid 394 and name CB)	16.57	0.67	0.66
	assign (segid 3A4 and resid 308 and name CB) (segid 3A4 and resid 395 and name CA)	16.19	0.72	0.72
	assign (segid 3A4 and resid 308 and name CB) (segid 3A4 and resid 396 and name CA)	16.74	0.57	0.57
	assign (segid 3A4 and resid 308 and name CB) (segid 3A4 and resid 396 and name CB)	18.06	0.57	0.56
	assign (segid 3A4 and resid 308 and name CB) (segid 3A4 and resid 397 and name CA)	14.22	0.60	0.61
70	assign (segid 3A4 and resid 308 and name CB) (segid 3A4 and resid 397 and name CB)	14.35	0.62	0.62
	assign (segid 3A4 and resid 308 and name CB) (segid 3A4 and resid 398 and name CA)	11.35	0.64	0.63
	assign (segid 3A4 and resid 308 and name CB) (segid 3A4 and resid 398 and name CB)	11.42	0.69	0.70
	assign (segid 3A4 and resid 308 and name CB) (segid 3A4 and resid 399 and name CA)	12.83	0.52	0.52
	assign (segid 3A4 and resid 308 and name CB) (segid 3A4 and resid 399 and name CB)	14.31	0.52	0.51
75	assign (segid 3A4 and resid 308 and name CB) (segid 3A4 and resid 400 and name CA)	13.22	0.51	0.50
	assign (segid 3A4 and resid 308 and name CB) (segid 3A4 and resid 400 and name CB)	14.12	0.46	0.45
	assign (segid 3A4 and resid 308 and name CB) (segid 3A4 and resid 401 and name CA)	9.73	0.49	0.48
	assign (segid 3A4 and resid 308 and name CB) (segid 3A4 and resid 402 and name CA)	8.45	0.50	0.51
	assign (segid 3A4 and resid 308 and name CB) (segid 3A4 and resid 402 and name CB)	8.82	0.46	0.46
80	assign (segid 3A4 and resid 308 and name CB) (segid 3A4 and resid 403 and name CA)	11.62	0.52	0.52
	assign (segid 3A4 and resid 308 and name CB) (segid 3A4 and resid 403 and name CB)	13.00	0.52	0.53
	assign (segid 3A4 and resid 308 and name CB) (segid 3A4 and resid 404 and name CA)	11.55	0.73	0.73

	assign (segid 3A4 and resid 308 and name CB)	(segid 3A4 and resid 404 and name CB)	11.70	0.83	0.82
	assign (segid 3A4 and resid 308 and name CB)	(segid 3A4 and resid 405 and name CA)	8.36	0.71	0.70
	assign (segid 3A4 and resid 308 and name CB)	(segid 3A4 and resid 405 and name CB)	6.95	0.72	0.71
	assign (segid 3A4 and resid 308 and name CB)	(segid 3A4 and resid 406 and name CA)	9.45	0.38	0.38
5	assign (segid 3A4 and resid 308 and name CB)	(segid 3A4 and resid 407 and name CA)	12.85	0.48	0.48
	assign (segid 3A4 and resid 308 and name CB)	(segid 3A4 and resid 407 and name CB)	13.79	0.53	0.54
	assign (segid 3A4 and resid 308 and name CB)	(segid 3A4 and resid 408 and name CA)	12.58	0.59	0.59
	assign (segid 3A4 and resid 308 and name CB)	(segid 3A4 and resid 408 and name CB)	11.96	0.69	0.70
	assign (segid 3A4 and resid 308 and name CB)	(segid 3A4 and resid 409 and name CA)	11.19	0.57	0.57
10	assign (segid 3A4 and resid 308 and name CB)	(segid 3A4 and resid 409 and name CB)	9.87	0.59	0.59
	assign (segid 3A4 and resid 308 and name CB)	(segid 3A4 and resid 410 and name CA)	13.63	0.31	0.32
	assign (segid 3A4 and resid 308 and name CB)	(segid 3A4 and resid 411 and name CA)	16.32	0.49	0.49
	assign (segid 3A4 and resid 308 and name CB)	(segid 3A4 and resid 411 and name CB)	16.68	0.63	0.64
	assign (segid 3A4 and resid 308 and name CB)	(segid 3A4 and resid 412 and name CA)	15.91	0.63	0.64
15	assign (segid 3A4 and resid 308 and name CB)	(segid 3A4 and resid 413 and name CA)	16.42	1.00	1.01
	assign (segid 3A4 and resid 308 and name CB)	(segid 3A4 and resid 414 and name CA)	15.75	1.13	1.14
	assign (segid 3A4 and resid 308 and name CB)	(segid 3A4 and resid 415 and name CA)	17.34	1.03	1.04
	assign (segid 3A4 and resid 308 and name CB)	(segid 3A4 and resid 415 and name CB)	18.28	0.73	0.72
20	assign (segid 3A4 and resid 308 and name N)	(segid 3A4 and resid 308 and name C)	2.45	0.03	0.03
	assign (segid 3A4 and resid 308 and name N)	(segid 3A4 and resid 308 and name CA)	1.45	0.00	0.01
	assign (segid 3A4 and resid 308 and name N)	(segid 3A4 and resid 308 and name CB)	2.46	0.03	0.03
	assign (segid 3A4 and resid 308 and name N)	(segid 3A4 and resid 308 and name O)	3.47	0.03	0.03
	assign (segid 3A4 and resid 308 and name N)	(segid 3A4 and resid 309 and name C)	4.68	0.03	0.04
25	assign (segid 3A4 and resid 308 and name N)	(segid 3A4 and resid 309 and name CA)	4.23	0.07	0.07
	assign (segid 3A4 and resid 308 and name N)	(segid 3A4 and resid 309 and name CB)	5.00	0.10	0.11
	assign (segid 3A4 and resid 308 and name N)	(segid 3A4 and resid 309 and name N)	2.82	0.07	0.08
	assign (segid 3A4 and resid 308 and name N)	(segid 3A4 and resid 309 and name O)	5.75	0.04	0.04
	assign (segid 3A4 and resid 308 and name N)	(segid 3A4 and resid 310 and name C)	5.59	0.11	0.11
30	assign (segid 3A4 and resid 308 and name N)	(segid 3A4 and resid 310 and name CA)	5.29	0.12	0.11
	assign (segid 3A4 and resid 308 and name N)	(segid 3A4 and resid 310 and name CB)	5.34	0.17	0.16
	assign (segid 3A4 and resid 308 and name N)	(segid 3A4 and resid 310 and name N)	4.29	0.09	0.09
	assign (segid 3A4 and resid 308 and name N)	(segid 3A4 and resid 310 and name O)	6.80	0.11	0.10
	assign (segid 3A4 and resid 308 and name N)	(segid 3A4 and resid 311 and name C)	6.36	0.07	0.08
35	assign (segid 3A4 and resid 308 and name N)	(segid 3A4 and resid 311 and name CA)	5.58	0.12	0.11
	assign (segid 3A4 and resid 308 and name N)	(segid 3A4 and resid 311 and name CB)	5.06	0.12	0.11
	assign (segid 3A4 and resid 308 and name N)	(segid 3A4 and resid 311 and name CD)	7.49	0.14	0.13
	assign (segid 3A4 and resid 308 and name N)	(segid 3A4 and resid 311 and name CG)	6.30	0.11	0.11
	assign (segid 3A4 and resid 308 and name N)	(segid 3A4 and resid 311 and name N)	4.77	0.11	0.12
40	assign (segid 3A4 and resid 308 and name N)	(segid 3A4 and resid 311 and name O)	7.56	0.08	0.09
	assign (segid 3A4 and resid 308 and name N)	(segid 3A4 and resid 311 and name OE1)	7.60	0.17	0.17
	assign (segid 3A4 and resid 308 and name N)	(segid 3A4 and resid 312 and name CA)	7.16	0.07	0.07
	assign (segid 3A4 and resid 308 and name N)	(segid 3A4 and resid 312 and name CB)	6.98	0.13	0.13
	assign (segid 3A4 and resid 308 and name N)	(segid 3A4 and resid 312 and name N)	6.03	0.05	0.05
45	assign (segid 3A4 and resid 308 and name N)	(segid 3A4 and resid 364 and name C)	7.03	0.08	0.07
	assign (segid 3A4 and resid 308 and name N)	(segid 3A4 and resid 364 and name O)	6.98	0.16	0.17
	assign (segid 3A4 and resid 308 and name N)	(segid 3A4 and resid 365 and name C)	5.34	0.17	0.18
	assign (segid 3A4 and resid 308 and name N)	(segid 3A4 and resid 365 and name CA)	4.90	0.10	0.09
	assign (segid 3A4 and resid 308 and name N)	(segid 3A4 and resid 365 and name CB)	4.34	0.24	0.24
50	assign (segid 3A4 and resid 308 and name N)	(segid 3A4 and resid 365 and name N)	6.15	0.14	0.13
	assign (segid 3A4 and resid 308 and name N)	(segid 3A4 and resid 365 and name O)	4.82	0.35	0.34
	assign (segid 3A4 and resid 308 and name O)	(segid 3A4 and resid 308 and name CB)	3.36	0.05	0.05
	assign (segid 3A4 and resid 308 and name O)	(segid 3A4 and resid 309 and name C)	2.94	0.10	0.09
	assign (segid 3A4 and resid 308 and name O)	(segid 3A4 and resid 309 and name CA)	2.78	0.04	0.03
55	assign (segid 3A4 and resid 308 and name O)	(segid 3A4 and resid 309 and name CB)	4.29	0.03	0.03
	assign (segid 3A4 and resid 308 and name O)	(segid 3A4 and resid 309 and name N)	2.25	0.01	0.01
	assign (segid 3A4 and resid 308 and name O)	(segid 3A4 and resid 309 and name O)	3.39	0.10	0.09
	assign (segid 3A4 and resid 308 and name O)	(segid 3A4 and resid 310 and name C)	4.03	0.19	0.18
	assign (segid 3A4 and resid 308 and name O)	(segid 3A4 and resid 310 and name CA)	4.32	0.17	0.17
60	assign (segid 3A4 and resid 308 and name O)	(segid 3A4 and resid 310 and name CB)	5.28	0.18	0.18
	assign (segid 3A4 and resid 308 and name O)	(segid 3A4 and resid 310 and name N)	3.40	0.15	0.15
	assign (segid 3A4 and resid 308 and name O)	(segid 3A4 and resid 310 and name O)	4.92	0.19	0.19
	assign (segid 3A4 and resid 308 and name O)	(segid 3A4 and resid 311 and name C)	3.67	0.09	0.09
	assign (segid 3A4 and resid 308 and name O)	(segid 3A4 and resid 311 and name CA)	3.67	0.14	0.14
65	assign (segid 3A4 and resid 308 and name O)	(segid 3A4 and resid 311 and name CB)	3.70	0.13	0.12
	assign (segid 3A4 and resid 308 and name O)	(segid 3A4 and resid 311 and name CD)	6.13	0.12	0.11
	assign (segid 3A4 and resid 308 and name O)	(segid 3A4 and resid 311 and name CG)	4.78	0.09	0.09
	assign (segid 3A4 and resid 308 and name O)	(segid 3A4 and resid 311 and name N)	3.22	0.15	0.16
	assign (segid 3A4 and resid 308 and name O)	(segid 3A4 and resid 311 and name O)	4.83	0.08	0.08
70	assign (segid 3A4 and resid 308 and name O)	(segid 3A4 and resid 311 and name OE1)	6.41	0.15	0.14
	assign (segid 3A4 and resid 308 and name O)	(segid 3A4 and resid 312 and name C)	4.96	0.07	0.06
	assign (segid 3A4 and resid 308 and name O)	(segid 3A4 and resid 312 and name CA)	3.76	0.07	0.08
	assign (segid 3A4 and resid 308 and name O)	(segid 3A4 and resid 312 and name CB)	3.54	0.11	0.11
	assign (segid 3A4 and resid 308 and name O)	(segid 3A4 and resid 312 and name N)	2.87	0.07	0.06
75	assign (segid 3A4 and resid 308 and name O)	(segid 3A4 and resid 312 and name O)	6.07	0.08	0.08
	assign (segid 3A4 and resid 308 and name O)	(segid 3A4 and resid 313 and name C)	7.16	0.10	0.09
	assign (segid 3A4 and resid 308 and name O)	(segid 3A4 and resid 313 and name CA)	6.40	0.06	0.06
	assign (segid 3A4 and resid 308 and name O)	(segid 3A4 and resid 313 and name CB)	6.69	0.07	0.07
	assign (segid 3A4 and resid 308 and name O)	(segid 3A4 and resid 313 and name CG)	6.67	0.16	0.16
80	assign (segid 3A4 and resid 308 and name O)	(segid 3A4 and resid 313 and name N)	5.02	0.07	0.07
	assign (segid 3A4 and resid 308 and name O)	(segid 3A4 and resid 314 and name CB)	7.64	0.11	0.11
	assign (segid 3A4 and resid 308 and name O)	(segid 3A4 and resid 314 and name N)	6.75	0.09	0.08
	assign (segid 3A4 and resid 308 and name O)	(segid 3A4 and resid 315 and name N)	7.58	0.16	0.16
	assign (segid 3A4 and resid 308 and name O)	(segid 3A4 and resid 363 and name CG)	6.66	0.27	0.27

	assign (segid 3A4 and resid 308 and name O) (segid 3A4 and resid 364 and name C)	7.12	0.14	0.14
	assign (segid 3A4 and resid 308 and name O) (segid 3A4 and resid 364 and name O)	7.14	0.24	0.24
	assign (segid 3A4 and resid 308 and name O) (segid 3A4 and resid 365 and name C)	6.87	0.22	0.22
	assign (segid 3A4 and resid 308 and name O) (segid 3A4 and resid 365 and name CA)	5.85	0.15	0.15
	assign (segid 3A4 and resid 308 and name O) (segid 3A4 and resid 365 and name CB)	5.62	0.16	0.17
5	assign (segid 3A4 and resid 308 and name O) (segid 3A4 and resid 365 and name N)	6.55	0.10	0.10
	assign (segid 3A4 and resid 308 and name O) (segid 3A4 and resid 365 and name O)	6.74	0.30	0.30
	assign (segid 3A4 and resid 308 and name O) (segid 3A4 and resid 309 and name CB)	2.51	0.02	0.03
	assign (segid 3A4 and resid 309 and name C) (segid 3A4 and resid 309 and name O)	1.23	0.00	0.00
	assign (segid 3A4 and resid 309 and name C) (segid 3A4 and resid 310 and name C)	3.02	0.02	0.03
10	assign (segid 3A4 and resid 309 and name C) (segid 3A4 and resid 310 and name CA)	2.44	0.02	0.01
	assign (segid 3A4 and resid 309 and name C) (segid 3A4 and resid 310 and name CB)	3.70	0.02	0.02
	assign (segid 3A4 and resid 309 and name C) (segid 3A4 and resid 310 and name N)	1.33	0.00	0.01
	assign (segid 3A4 and resid 309 and name C) (segid 3A4 and resid 310 and name O)	3.85	0.07	0.07
	assign (segid 3A4 and resid 309 and name C) (segid 3A4 and resid 311 and name C)	4.53	0.04	0.03
15	assign (segid 3A4 and resid 309 and name C) (segid 3A4 and resid 311 and name CA)	4.46	0.03	0.04
	assign (segid 3A4 and resid 309 and name C) (segid 3A4 and resid 311 and name CB)	5.29	0.04	0.04
	assign (segid 3A4 and resid 309 and name C) (segid 3A4 and resid 311 and name CG)	7.61	0.04	0.04
	assign (segid 3A4 and resid 309 and name C) (segid 3A4 and resid 311 and name CD)	6.63	0.04	0.04
	assign (segid 3A4 and resid 309 and name C) (segid 3A4 and resid 311 and name N)	3.31	0.04	0.03
20	assign (segid 3A4 and resid 309 and name C) (segid 3A4 and resid 311 and name O)	5.64	0.04	0.04
	assign (segid 3A4 and resid 309 and name C) (segid 3A4 and resid 311 and name OE1)	7.44	0.05	0.05
	assign (segid 3A4 and resid 309 and name C) (segid 3A4 and resid 312 and name C)	4.89	0.06	0.07
	assign (segid 3A4 and resid 309 and name C) (segid 3A4 and resid 312 and name CA)	4.52	0.06	0.06
	assign (segid 3A4 and resid 309 and name C) (segid 3A4 and resid 312 and name CB)	4.29	0.13	0.13
25	assign (segid 3A4 and resid 309 and name C) (segid 3A4 and resid 312 and name N)	3.78	0.06	0.06
	assign (segid 3A4 and resid 309 and name C) (segid 3A4 and resid 312 and name O)	6.11	0.07	0.06
	assign (segid 3A4 and resid 309 and name C) (segid 3A4 and resid 313 and name C)	6.15	0.12	0.13
	assign (segid 3A4 and resid 309 and name C) (segid 3A4 and resid 313 and name CA)	5.16	0.12	0.12
	assign (segid 3A4 and resid 309 and name C) (segid 3A4 and resid 313 and name CB)	4.79	0.15	0.16
30	assign (segid 3A4 and resid 309 and name C) (segid 3A4 and resid 313 and name CG)	4.49	0.18	0.17
	assign (segid 3A4 and resid 309 and name C) (segid 3A4 and resid 313 and name N)	4.20	0.10	0.10
	assign (segid 3A4 and resid 309 and name C) (segid 3A4 and resid 313 and name O)	7.32	0.14	0.13
	assign (segid 3A4 and resid 309 and name C) (segid 3A4 and resid 314 and name CA)	7.30	0.08	0.07
	assign (segid 3A4 and resid 309 and name C) (segid 3A4 and resid 314 and name CB)	7.34	0.10	0.10
35	assign (segid 3A4 and resid 309 and name C) (segid 3A4 and resid 314 and name N)	6.02	0.09	0.08
	assign (segid 3A4 and resid 309 and name C) (segid 3A4 and resid 309 and name CB)	1.53	0.01	0.01
	assign (segid 3A4 and resid 309 and name CA) (segid 3A4 and resid 309 and name O)	2.40	0.01	0.00
	assign (segid 3A4 and resid 309 and name CA) (segid 3A4 and resid 310 and name C)	4.43	0.03	0.03
40	assign (segid 3A4 and resid 309 and name CA) (segid 3A4 and resid 310 and name CA)	3.83	0.03	0.03
	assign (segid 3A4 and resid 309 and name CA) (segid 3A4 and resid 310 and name CB)	4.88	0.04	0.03
	assign (segid 3A4 and resid 309 and name CA) (segid 3A4 and resid 310 and name N)	2.45	0.03	0.03
	assign (segid 3A4 and resid 309 and name CA) (segid 3A4 and resid 310 and name O)	5.32	0.08	0.07
	assign (segid 3A4 and resid 309 and name CA) (segid 3A4 and resid 311 and name C)	5.45	0.03	0.03
45	assign (segid 3A4 and resid 309 and name CA) (segid 3A4 and resid 311 and name CA)	5.46	0.03	0.03
	assign (segid 3A4 and resid 309 and name CA) (segid 3A4 and resid 311 and name CB)	5.98	0.04	0.03
	assign (segid 3A4 and resid 309 and name CA) (segid 3A4 and resid 311 and name CG)	7.27	0.03	0.02
	assign (segid 3A4 and resid 309 and name CA) (segid 3A4 and resid 311 and name N)	4.41	0.04	0.04
	assign (segid 3A4 and resid 309 and name CA) (segid 3A4 and resid 311 and name O)	6.59	0.05	0.05
50	assign (segid 3A4 and resid 309 and name CA) (segid 3A4 and resid 312 and name C)	5.70	0.08	0.08
	assign (segid 3A4 and resid 309 and name CA) (segid 3A4 and resid 312 and name CA)	5.06	0.08	0.08
	assign (segid 3A4 and resid 309 and name CA) (segid 3A4 and resid 312 and name CB)	4.41	0.16	0.17
	assign (segid 3A4 and resid 309 and name CA) (segid 3A4 and resid 312 and name N)	4.50	0.08	0.07
	assign (segid 3A4 and resid 309 and name CA) (segid 3A4 and resid 312 and name O)	6.88	0.08	0.08
55	assign (segid 3A4 and resid 309 and name CA) (segid 3A4 and resid 313 and name C)	7.41	0.12	0.12
	assign (segid 3A4 and resid 309 and name CA) (segid 3A4 and resid 313 and name CA)	6.29	0.12	0.12
	assign (segid 3A4 and resid 309 and name CA) (segid 3A4 and resid 313 and name CB)	6.01	0.16	0.15
	assign (segid 3A4 and resid 309 and name CA) (segid 3A4 and resid 313 and name CG)	5.44	0.23	0.22
	assign (segid 3A4 and resid 309 and name CA) (segid 3A4 and resid 313 and name N)	5.23	0.10	0.10
60	assign (segid 3A4 and resid 309 and name CA) (segid 3A4 and resid 314 and name CA)	8.65	0.07	0.08
	assign (segid 3A4 and resid 309 and name CA) (segid 3A4 and resid 314 and name CB)	8.72	0.10	0.10
	assign (segid 3A4 and resid 309 and name CA) (segid 3A4 and resid 314 and name N)	7.35	0.09	0.08
	assign (segid 3A4 and resid 309 and name CA) (segid 3A4 and resid 315 and name CA)	9.92	0.09	0.09
	assign (segid 3A4 and resid 309 and name CA) (segid 3A4 and resid 315 and name CB)	9.54	0.17	0.18
65	assign (segid 3A4 and resid 309 and name CA) (segid 3A4 and resid 316 and name CA)	10.50	0.23	0.23
	assign (segid 3A4 and resid 309 and name CA) (segid 3A4 and resid 317 and name CA)	11.50	0.55	0.55
	assign (segid 3A4 and resid 309 and name CA) (segid 3A4 and resid 318 and name CA)	12.92	0.68	0.69
	assign (segid 3A4 and resid 309 and name CA) (segid 3A4 and resid 318 and name CB)	12.26	0.70	0.69
	assign (segid 3A4 and resid 309 and name CA) (segid 3A4 and resid 319 and name CA)	15.51	0.62	0.63
70	assign (segid 3A4 and resid 309 and name CA) (segid 3A4 and resid 319 and name CB)	15.42	0.57	0.57
	assign (segid 3A4 and resid 309 and name CA) (segid 3A4 and resid 347 and name CA)	16.73	0.42	0.43
	assign (segid 3A4 and resid 309 and name CA) (segid 3A4 and resid 347 and name CB)	15.96	0.47	0.46
	assign (segid 3A4 and resid 309 and name CA) (segid 3A4 and resid 348 and name CA)	15.75	0.55	0.54
	assign (segid 3A4 and resid 309 and name CA) (segid 3A4 and resid 349 and name CA)	18.41	0.50	0.49
75	assign (segid 3A4 and resid 309 and name CA) (segid 3A4 and resid 350 and name CA)	17.43	0.25	0.25
	assign (segid 3A4 and resid 309 and name CA) (segid 3A4 and resid 350 and name CB)	17.28	0.37	0.37
	assign (segid 3A4 and resid 309 and name CA) (segid 3A4 and resid 351 and name CA)	14.05	0.16	0.16
	assign (segid 3A4 and resid 309 and name CA) (segid 3A4 and resid 352 and name CA)	16.12	0.28	0.28
	assign (segid 3A4 and resid 309 and name CA) (segid 3A4 and resid 352 and name CB)	16.52	0.26	0.27
80	assign (segid 3A4 and resid 309 and name CA) (segid 3A4 and resid 353 and name CA)	18.87	0.33	0.34
	assign (segid 3A4 and resid 309 and name CA) (segid 3A4 and resid 353 and name CB)	19.15	0.38	0.37
	assign (segid 3A4 and resid 309 and name CA) (segid 3A4 and resid 356 and name CA)	18.39	0.50	0.49

	assign	(segid 3A4 and resid 309 and name CA)	(segid 3A4 and resid 356 and name CB)	17.78	0.46	0.46
	assign	(segid 3A4 and resid 309 and name CA)	(segid 3A4 and resid 357 and name CA)	16.11	0.43	0.43
	assign	(segid 3A4 and resid 309 and name CA)	(segid 3A4 and resid 357 and name CB)	14.94	0.48	0.48
	assign	(segid 3A4 and resid 309 and name CA)	(segid 3A4 and resid 359 and name CA)	17.86	0.20	0.21
5	assign	(segid 3A4 and resid 309 and name CA)	(segid 3A4 and resid 359 and name CB)	17.83	0.23	0.23
	assign	(segid 3A4 and resid 309 and name CA)	(segid 3A4 and resid 360 and name CA)	15.65	0.14	0.14
	assign	(segid 3A4 and resid 309 and name CA)	(segid 3A4 and resid 360 and name CB)	16.45	0.19	0.19
	assign	(segid 3A4 and resid 309 and name CA)	(segid 3A4 and resid 361 and name CA)	15.89	0.23	0.23
	assign	(segid 3A4 and resid 309 and name CA)	(segid 3A4 and resid 361 and name CB)	17.26	0.27	0.27
10	assign	(segid 3A4 and resid 309 and name CA)	(segid 3A4 and resid 362 and name CA)	14.50	0.16	0.16
	assign	(segid 3A4 and resid 309 and name CA)	(segid 3A4 and resid 362 and name CB)	15.25	0.13	0.13
	assign	(segid 3A4 and resid 309 and name CA)	(segid 3A4 and resid 363 and name CA)	11.04	0.15	0.14
	assign	(segid 3A4 and resid 309 and name CA)	(segid 3A4 and resid 363 and name CB)	10.70	0.23	0.23
	assign	(segid 3A4 and resid 309 and name CA)	(segid 3A4 and resid 364 and name CA)	10.77	0.07	0.07
15	assign	(segid 3A4 and resid 309 and name CA)	(segid 3A4 and resid 364 and name CB)	12.04	0.07	0.07
	assign	(segid 3A4 and resid 309 and name CA)	(segid 3A4 and resid 365 and name CA)	8.14	0.13	0.13
	assign	(segid 3A4 and resid 309 and name CA)	(segid 3A4 and resid 365 and name CB)	7.81	0.16	0.16
	assign	(segid 3A4 and resid 309 and name CA)	(segid 3A4 and resid 381 and name CA)	12.01	0.36	0.36
	assign	(segid 3A4 and resid 309 and name CA)	(segid 3A4 and resid 382 and name CA)	13.60	0.15	0.16
20	assign	(segid 3A4 and resid 309 and name CA)	(segid 3A4 and resid 382 and name CB)	15.06	0.18	0.19
	assign	(segid 3A4 and resid 309 and name CA)	(segid 3A4 and resid 383 and name CA)	11.39	0.26	0.27
	assign	(segid 3A4 and resid 309 and name CA)	(segid 3A4 and resid 384 and name CA)	12.71	0.39	0.40
	assign	(segid 3A4 and resid 309 and name CA)	(segid 3A4 and resid 384 and name CB)	12.19	0.46	0.45
	assign	(segid 3A4 and resid 309 and name CA)	(segid 3A4 and resid 385 and name CA)	16.09	0.33	0.33
25	assign	(segid 3A4 and resid 309 and name CA)	(segid 3A4 and resid 386 and name CA)	18.27	0.38	0.38
	assign	(segid 3A4 and resid 309 and name CA)	(segid 3A4 and resid 390 and name CA)	17.93	0.50	0.51
	assign	(segid 3A4 and resid 309 and name CA)	(segid 3A4 and resid 390 and name CB)	17.63	0.46	0.47
	assign	(segid 3A4 and resid 309 and name CA)	(segid 3A4 and resid 391 and name CA)	16.02	0.54	0.53
	assign	(segid 3A4 and resid 309 and name CA)	(segid 3A4 and resid 391 and name CB)	14.62	0.53	0.52
30	assign	(segid 3A4 and resid 309 and name CA)	(segid 3A4 and resid 392 and name CA)	17.58	0.55	0.55
	assign	(segid 3A4 and resid 309 and name CA)	(segid 3A4 and resid 393 and name CA)	15.09	0.57	0.58
	assign	(segid 3A4 and resid 309 and name CA)	(segid 3A4 and resid 394 and name CA)	12.04	0.62	0.63
	assign	(segid 3A4 and resid 309 and name CA)	(segid 3A4 and resid 394 and name CB)	12.26	0.70	0.71
	assign	(segid 3A4 and resid 309 and name CA)	(segid 3A4 and resid 395 and name CA)	12.29	0.71	0.70
35	assign	(segid 3A4 and resid 309 and name CA)	(segid 3A4 and resid 396 and name CA)	12.90	0.56	0.56
	assign	(segid 3A4 and resid 309 and name CA)	(segid 3A4 and resid 396 and name CB)	14.16	0.56	0.57
	assign	(segid 3A4 and resid 309 and name CA)	(segid 3A4 and resid 397 and name CA)	10.13	0.61	0.60
	assign	(segid 3A4 and resid 309 and name CA)	(segid 3A4 and resid 397 and name CB)	10.08	0.64	0.64
40	assign	(segid 3A4 and resid 309 and name CA)	(segid 3A4 and resid 398 and name CA)	7.47	0.62	0.61
	assign	(segid 3A4 and resid 309 and name CA)	(segid 3A4 and resid 398 and name CB)	7.57	0.68	0.68
	assign	(segid 3A4 and resid 309 and name CA)	(segid 3A4 and resid 398 and name O)	7.10	0.51	0.52
	assign	(segid 3A4 and resid 309 and name CA)	(segid 3A4 and resid 399 and name CA)	9.82	0.47	0.47
	assign	(segid 3A4 and resid 309 and name CA)	(segid 3A4 and resid 399 and name CB)	11.29	0.48	0.48
	assign	(segid 3A4 and resid 309 and name CA)	(segid 3A4 and resid 400 and name CA)	10.30	0.40	0.41
45	assign	(segid 3A4 and resid 309 and name CA)	(segid 3A4 and resid 400 and name CB)	10.97	0.35	0.34
	assign	(segid 3A4 and resid 309 and name CA)	(segid 3A4 and resid 401 and name C)	6.60	0.36	0.36
	assign	(segid 3A4 and resid 309 and name CA)	(segid 3A4 and resid 401 and name CA)	6.90	0.37	0.37
	assign	(segid 3A4 and resid 309 and name CA)	(segid 3A4 and resid 401 and name O)	6.74	0.34	0.35
	assign	(segid 3A4 and resid 309 and name CA)	(segid 3A4 and resid 402 and name CA)	6.80	0.36	0.36
50	assign	(segid 3A4 and resid 309 and name CA)	(segid 3A4 and resid 402 and name CB)	7.05	0.37	0.37
	assign	(segid 3A4 and resid 309 and name CA)	(segid 3A4 and resid 402 and name N)	6.60	0.37	0.38
	assign	(segid 3A4 and resid 309 and name CA)	(segid 3A4 and resid 403 and name CA)	10.46	0.34	0.35
	assign	(segid 3A4 and resid 309 and name CA)	(segid 3A4 and resid 403 and name CB)	11.51	0.34	0.35
55	assign	(segid 3A4 and resid 309 and name CA)	(segid 3A4 and resid 404 and name CA)	10.58	0.41	0.41
	assign	(segid 3A4 and resid 309 and name CA)	(segid 3A4 and resid 404 and name CB)	10.33	0.51	0.51
	assign	(segid 3A4 and resid 309 and name CA)	(segid 3A4 and resid 405 and name CA)	8.56	0.24	0.25
	assign	(segid 3A4 and resid 309 and name CA)	(segid 3A4 and resid 405 and name CB)	7.12	0.23	0.24
	assign	(segid 3A4 and resid 309 and name CA)	(segid 3A4 and resid 406 and name CA)	10.42	0.41	0.41
60	assign	(segid 3A4 and resid 309 and name CA)	(segid 3A4 and resid 407 and name CA)	13.55	0.31	0.30
	assign	(segid 3A4 and resid 309 and name CA)	(segid 3A4 and resid 407 and name CB)	14.06	0.31	0.31
	assign	(segid 3A4 and resid 309 and name CA)	(segid 3A4 and resid 408 and name CA)	13.56	0.19	0.19
	assign	(segid 3A4 and resid 309 and name CA)	(segid 3A4 and resid 408 and name CB)	12.74	0.22	0.23
	assign	(segid 3A4 and resid 309 and name CA)	(segid 3A4 and resid 409 and name CA)	13.37	0.53	0.53
	assign	(segid 3A4 and resid 309 and name CA)	(segid 3A4 and resid 409 and name CB)	12.30	0.66	0.66
65	assign	(segid 3A4 and resid 309 and name CA)	(segid 3A4 and resid 410 and name CA)	15.85	0.44	0.43
	assign	(segid 3A4 and resid 309 and name CA)	(segid 3A4 and resid 411 and name CA)	18.14	0.32	0.31
	assign	(segid 3A4 and resid 309 and name CA)	(segid 3A4 and resid 411 and name CB)	18.14	0.38	0.39
	assign	(segid 3A4 and resid 309 and name CA)	(segid 3A4 and resid 412 and name CA)	18.05	0.48	0.48
	assign	(segid 3A4 and resid 309 and name CA)	(segid 3A4 and resid 414 and name CA)	17.96	0.93	0.93
70	assign	(segid 3A4 and resid 309 and name CA)	(segid 3A4 and resid 433 and name CA)	16.64	0.82	0.81
	assign	(segid 3A4 and resid 309 and name CA)	(segid 3A4 and resid 434 and name CA)	15.83	1.02	1.01
	assign	(segid 3A4 and resid 309 and name CA)	(segid 3A4 and resid 435 and name CA)	16.50	0.93	0.93
	assign	(segid 3A4 and resid 309 and name CA)	(segid 3A4 and resid 438 and name CA)	18.70	0.80	0.80
	assign	(segid 3A4 and resid 309 and name CB)	(segid 3A4 and resid 310 and name C)	5.45	0.04	0.04
75	assign	(segid 3A4 and resid 309 and name CB)	(segid 3A4 and resid 310 and name CA)	4.50	0.04	0.03
	assign	(segid 3A4 and resid 309 and name CB)	(segid 3A4 and resid 310 and name CB)	5.35	0.03	0.04
	assign	(segid 3A4 and resid 309 and name CB)	(segid 3A4 and resid 310 and name N)	3.16	0.04	0.04
	assign	(segid 3A4 and resid 309 and name CB)	(segid 3A4 and resid 310 and name O)	6.30	0.09	0.08
	assign	(segid 3A4 and resid 309 and name CB)	(segid 3A4 and resid 311 and name C)	6.88	0.04	0.05
80	assign	(segid 3A4 and resid 309 and name CB)	(segid 3A4 and resid 311 and name CA)	6.84	0.04	0.03
	assign	(segid 3A4 and resid 309 and name CB)	(segid 3A4 and resid 311 and name CB)	7.41	0.04	0.03
	assign	(segid 3A4 and resid 309 and name CB)	(segid 3A4 and resid 311 and name N)	5.66	0.04	0.03
	assign	(segid 3A4 and resid 309 and name CB)	(segid 3A4 and resid 312 and name C)	6.87	0.09	0.10

	assign (segid 3A4 and resid 309 and name CB) (segid 3A4 and resid 312 and name CA)	6.42	0.10	0.10
	assign (segid 3A4 and resid 309 and name CB) (segid 3A4 and resid 312 and name CB)	5.67	0.19	0.19
	assign (segid 3A4 and resid 309 and name CB) (segid 3A4 and resid 312 and name N)	5.95	0.09	0.09
	assign (segid 3A4 and resid 309 and name CB) (segid 3A4 and resid 313 and name CA)	7.09	0.15	0.14
	assign (segid 3A4 and resid 309 and name CB) (segid 3A4 and resid 313 and name CB)	6.53	0.18	0.18
5	assign (segid 3A4 and resid 309 and name CB) (segid 3A4 and resid 313 and name CG)	5.68	0.24	0.24
	assign (segid 3A4 and resid 309 and name CB) (segid 3A4 and resid 313 and name N)	6.24	0.11	0.11
	assign (segid 3A4 and resid 309 and name CB) (segid 3A4 and resid 314 and name CA)	9.71	0.08	0.07
	assign (segid 3A4 and resid 309 and name CB) (segid 3A4 and resid 314 and name CB)	9.83	0.09	0.09
	assign (segid 3A4 and resid 309 and name CB) (segid 3A4 and resid 315 and name CA)	11.24	0.06	0.06
10	assign (segid 3A4 and resid 309 and name CB) (segid 3A4 and resid 315 and name CB)	10.96	0.15	0.14
	assign (segid 3A4 and resid 309 and name CB) (segid 3A4 and resid 316 and name CA)	11.57	0.25	0.25
	assign (segid 3A4 and resid 309 and name CB) (segid 3A4 and resid 317 and name CA)	12.26	0.67	0.67
	assign (segid 3A4 and resid 309 and name CB) (segid 3A4 and resid 318 and name CA)	13.41	0.81	0.81
	assign (segid 3A4 and resid 309 and name CB) (segid 3A4 and resid 318 and name CB)	12.63	0.84	0.85
15	assign (segid 3A4 and resid 309 and name CB) (segid 3A4 and resid 319 and name CA)	15.83	0.74	0.74
	assign (segid 3A4 and resid 309 and name CB) (segid 3A4 and resid 319 and name CB)	15.61	0.69	0.68
	assign (segid 3A4 and resid 309 and name CB) (segid 3A4 and resid 347 and name CA)	17.33	0.45	0.46
	assign (segid 3A4 and resid 309 and name CB) (segid 3A4 and resid 347 and name CB)	16.46	0.49	0.48
20	assign (segid 3A4 and resid 309 and name CB) (segid 3A4 and resid 348 and name CA)	16.61	0.58	0.59
	assign (segid 3A4 and resid 309 and name CB) (segid 3A4 and resid 350 and name CA)	18.27	0.30	0.30
	assign (segid 3A4 and resid 309 and name CB) (segid 3A4 and resid 350 and name CB)	18.01	0.42	0.42
	assign (segid 3A4 and resid 309 and name CB) (segid 3A4 and resid 351 and name CA)	15.03	0.20	0.19
	assign (segid 3A4 and resid 309 and name CB) (segid 3A4 and resid 352 and name CA)	17.31	0.29	0.29
	assign (segid 3A4 and resid 309 and name CB) (segid 3A4 and resid 352 and name CB)	17.75	0.28	0.27
25	assign (segid 3A4 and resid 309 and name CB) (segid 3A4 and resid 356 and name CB)	18.68	0.47	0.48
	assign (segid 3A4 and resid 309 and name CB) (segid 3A4 and resid 357 and name CA)	17.26	0.42	0.41
	assign (segid 3A4 and resid 309 and name CB) (segid 3A4 and resid 357 and name CB)	16.11	0.47	0.48
	assign (segid 3A4 and resid 309 and name CB) (segid 3A4 and resid 359 and name CA)	19.29	0.21	0.21
	assign (segid 3A4 and resid 309 and name CB) (segid 3A4 and resid 359 and name CB)	19.28	0.24	0.24
30	assign (segid 3A4 and resid 309 and name CB) (segid 3A4 and resid 360 and name CA)	17.05	0.15	0.14
	assign (segid 3A4 and resid 309 and name CB) (segid 3A4 and resid 360 and name CB)	17.80	0.20	0.19
	assign (segid 3A4 and resid 309 and name CB) (segid 3A4 and resid 361 and name CA)	17.38	0.24	0.24
	assign (segid 3A4 and resid 309 and name CB) (segid 3A4 and resid 361 and name CB)	18.75	0.28	0.28
35	assign (segid 3A4 and resid 309 and name CB) (segid 3A4 and resid 362 and name CA)	16.03	0.17	0.17
	assign (segid 3A4 and resid 309 and name CB) (segid 3A4 and resid 362 and name CB)	16.77	0.12	0.12
	assign (segid 3A4 and resid 309 and name CB) (segid 3A4 and resid 363 and name CA)	12.58	0.16	0.15
	assign (segid 3A4 and resid 309 and name CB) (segid 3A4 and resid 363 and name CB)	12.23	0.23	0.24
	assign (segid 3A4 and resid 309 and name CB) (segid 3A4 and resid 364 and name CA)	12.20	0.06	0.06
	assign (segid 3A4 and resid 309 and name CB) (segid 3A4 and resid 364 and name CB)	13.44	0.07	0.07
40	assign (segid 3A4 and resid 309 and name CB) (segid 3A4 and resid 365 and name CA)	9.37	0.11	0.11
	assign (segid 3A4 and resid 309 and name CB) (segid 3A4 and resid 365 and name CB)	8.96	0.15	0.16
	assign (segid 3A4 and resid 309 and name CB) (segid 3A4 and resid 381 and name CA)	12.55	0.33	0.33
	assign (segid 3A4 and resid 309 and name CB) (segid 3A4 and resid 382 and name CA)	13.93	0.14	0.14
	assign (segid 3A4 and resid 309 and name CB) (segid 3A4 and resid 382 and name CB)	15.42	0.15	0.16
45	assign (segid 3A4 and resid 309 and name CB) (segid 3A4 and resid 383 and name CA)	11.68	0.29	0.28
	assign (segid 3A4 and resid 309 and name CB) (segid 3A4 and resid 384 and name CA)	12.54	0.36	0.36
	assign (segid 3A4 and resid 309 and name CB) (segid 3A4 and resid 384 and name CB)	11.86	0.42	0.42
	assign (segid 3A4 and resid 309 and name CB) (segid 3A4 and resid 385 and name CA)	16.04	0.29	0.30
	assign (segid 3A4 and resid 309 and name CB) (segid 3A4 and resid 386 and name CA)	18.16	0.30	0.30
50	assign (segid 3A4 and resid 309 and name CB) (segid 3A4 and resid 390 and name CA)	17.49	0.51	0.51
	assign (segid 3A4 and resid 309 and name CB) (segid 3A4 and resid 390 and name CB)	17.17	0.48	0.47
	assign (segid 3A4 and resid 309 and name CB) (segid 3A4 and resid 391 and name CA)	15.41	0.55	0.55
	assign (segid 3A4 and resid 309 and name CB) (segid 3A4 and resid 391 and name CB)	14.04	0.52	0.53
	assign (segid 3A4 and resid 309 and name CB) (segid 3A4 and resid 392 and name CA)	16.70	0.56	0.55
55	assign (segid 3A4 and resid 309 and name CB) (segid 3A4 and resid 392 and name CB)	18.04	0.56	0.56
	assign (segid 3A4 and resid 309 and name CB) (segid 3A4 and resid 393 and name CA)	14.09	0.58	0.58
	assign (segid 3A4 and resid 309 and name CB) (segid 3A4 and resid 394 and name CA)	11.10	0.63	0.64
	assign (segid 3A4 and resid 309 and name CB) (segid 3A4 and resid 394 and name CB)	11.41	0.69	0.70
60	assign (segid 3A4 and resid 309 and name CB) (segid 3A4 and resid 395 and name CA)	11.02	0.71	0.72
	assign (segid 3A4 and resid 309 and name CB) (segid 3A4 and resid 396 and name CA)	11.58	0.57	0.56
	assign (segid 3A4 and resid 309 and name CB) (segid 3A4 and resid 396 and name CB)	12.88	0.56	0.56
	assign (segid 3A4 and resid 309 and name CB) (segid 3A4 and resid 397 and name CA)	9.03	0.61	0.60
	assign (segid 3A4 and resid 309 and name CB) (segid 3A4 and resid 397 and name CB)	9.13	0.64	0.64
65	assign (segid 3A4 and resid 309 and name CB) (segid 3A4 and resid 398 and name C)	6.39	0.57	0.56
	assign (segid 3A4 and resid 309 and name CB) (segid 3A4 and resid 398 and name CA)	6.14	0.64	0.63
	assign (segid 3A4 and resid 309 and name CB) (segid 3A4 and resid 398 and name CB)	6.26	0.70	0.70
	assign (segid 3A4 and resid 309 and name CB) (segid 3A4 and resid 398 and name CG)	6.13	0.68	0.68
	assign (segid 3A4 and resid 309 and name CB) (segid 3A4 and resid 398 and name O)	5.63	0.53	0.53
70	assign (segid 3A4 and resid 309 and name CB) (segid 3A4 and resid 399 and name CA)	8.33	0.48	0.47
	assign (segid 3A4 and resid 309 and name CB) (segid 3A4 and resid 399 and name CB)	9.79	0.49	0.48
	assign (segid 3A4 and resid 309 and name CB) (segid 3A4 and resid 400 and name CA)	9.04	0.40	0.39
	assign (segid 3A4 and resid 309 and name CB) (segid 3A4 and resid 400 and name CB)	9.78	0.36	0.35
	assign (segid 3A4 and resid 309 and name CB) (segid 3A4 and resid 401 and name C)	5.50	0.34	0.34
	assign (segid 3A4 and resid 309 and name CB) (segid 3A4 and resid 401 and name CA)	5.85	0.34	0.35
75	assign (segid 3A4 and resid 309 and name CB) (segid 3A4 and resid 401 and name N)	6.79	0.40	0.41
	assign (segid 3A4 and resid 309 and name CB) (segid 3A4 and resid 401 and name O)	5.83	0.33	0.33
	assign (segid 3A4 and resid 309 and name CB) (segid 3A4 and resid 402 and name C)	6.96	0.35	0.35
	assign (segid 3A4 and resid 309 and name CB) (segid 3A4 and resid 402 and name CA)	5.54	0.37	0.36
	assign (segid 3A4 and resid 309 and name CB) (segid 3A4 and resid 402 and name CB)	5.67	0.38	0.38
80	assign (segid 3A4 and resid 309 and name CB) (segid 3A4 and resid 402 and name N)	5.32	0.36	0.36
	assign (segid 3A4 and resid 309 and name CB) (segid 3A4 and resid 403 and name CA)	9.26	0.34	0.35
	assign (segid 3A4 and resid 309 and name CB) (segid 3A4 and resid 403 and name CB)	10.24	0.34	0.34

	assign (segid 3A4 and resid 309 and name CD)	(segid 3A4 and resid 404 and name CA)	9.75	0.35	0.36
	assign (segid 3A4 and resid 309 and name CB)	(segid 3A4 and resid 404 and name CB)	9.57	0.43	0.43
	assign (segid 3A4 and resid 309 and name CB)	(segid 3A4 and resid 405 and name CA)	8.12	0.28	0.27
	assign (segid 3A4 and resid 309 and name CB)	(segid 3A4 and resid 405 and name CB)	6.78	0.26	0.27
5	assign (segid 3A4 and resid 309 and name CB)	(segid 3A4 and resid 406 and name CA)	9.77	0.48	0.48
	assign (segid 3A4 and resid 309 and name CB)	(segid 3A4 and resid 407 and name CA)	12.87	0.38	0.37
	assign (segid 3A4 and resid 309 and name CB)	(segid 3A4 and resid 407 and name CB)	13.27	0.36	0.36
	assign (segid 3A4 and resid 309 and name CB)	(segid 3A4 and resid 408 and name CA)	13.23	0.26	0.27
	assign (segid 3A4 and resid 309 and name CB)	(segid 3A4 and resid 408 and name CB)	12.51	0.28	0.27
	assign (segid 3A4 and resid 309 and name CB)	(segid 3A4 and resid 409 and name CA)	13.31	0.58	0.57
10	assign (segid 3A4 and resid 309 and name CB)	(segid 3A4 and resid 409 and name CB)	12.31	0.72	0.73
	assign (segid 3A4 and resid 309 and name CB)	(segid 3A4 and resid 410 and name CA)	15.55	0.52	0.52
	assign (segid 3A4 and resid 309 and name CB)	(segid 3A4 and resid 411 and name CA)	17.84	0.38	0.38
	assign (segid 3A4 and resid 309 and name CB)	(segid 3A4 and resid 411 and name CB)	17.78	0.44	0.43
	assign (segid 3A4 and resid 309 and name CB)	(segid 3A4 and resid 412 and name CA)	18.06	0.49	0.48
15	assign (segid 3A4 and resid 309 and name CB)	(segid 3A4 and resid 433 and name CA)	17.23	0.90	0.89
	assign (segid 3A4 and resid 309 and name CB)	(segid 3A4 and resid 434 and name CA)	16.40	1.06	1.06
	assign (segid 3A4 and resid 309 and name CB)	(segid 3A4 and resid 435 and name CA)	17.16	0.92	0.92
	assign (segid 3A4 and resid 309 and name N)	(segid 3A4 and resid 309 and name C)	2.45	0.02	0.02
	assign (segid 3A4 and resid 309 and name N)	(segid 3A4 and resid 309 and name CA)	1.47	0.01	0.01
20	assign (segid 3A4 and resid 309 and name N)	(segid 3A4 and resid 309 and name CB)	2.49	0.02	0.01
	assign (segid 3A4 and resid 309 and name N)	(segid 3A4 and resid 309 and name O)	3.48	0.02	0.02
	assign (segid 3A4 and resid 309 and name N)	(segid 3A4 and resid 310 and name C)	4.70	0.06	0.06
	assign (segid 3A4 and resid 309 and name N)	(segid 3A4 and resid 310 and name CA)	4.22	0.07	0.06
	assign (segid 3A4 and resid 309 and name N)	(segid 3A4 and resid 310 and name CB)	4.96	0.07	0.08
25	assign (segid 3A4 and resid 309 and name N)	(segid 3A4 and resid 310 and name N)	2.81	0.07	0.08
	assign (segid 3A4 and resid 309 and name N)	(segid 3A4 and resid 310 and name O)	5.77	0.08	0.08
	assign (segid 3A4 and resid 309 and name N)	(segid 3A4 and resid 311 and name C)	5.55	0.03	0.02
	assign (segid 3A4 and resid 309 and name N)	(segid 3A4 and resid 311 and name CA)	5.31	0.06	0.06
	assign (segid 3A4 and resid 309 and name N)	(segid 3A4 and resid 311 and name CB)	5.45	0.05	0.05
30	assign (segid 3A4 and resid 309 and name N)	(segid 3A4 and resid 311 and name CG)	6.75	0.05	0.06
	assign (segid 3A4 and resid 309 and name N)	(segid 3A4 and resid 311 and name N)	4.31	0.06	0.06
	assign (segid 3A4 and resid 309 and name N)	(segid 3A4 and resid 311 and name O)	6.76	0.03	0.03
	assign (segid 3A4 and resid 309 and name N)	(segid 3A4 and resid 312 and name C)	6.43	0.06	0.07
	assign (segid 3A4 and resid 309 and name N)	(segid 3A4 and resid 312 and name CA)	5.52	0.08	0.08
35	assign (segid 3A4 and resid 309 and name N)	(segid 3A4 and resid 312 and name CB)	4.98	0.16	0.16
	assign (segid 3A4 and resid 309 and name N)	(segid 3A4 and resid 312 and name N)	4.74	0.05	0.04
	assign (segid 3A4 and resid 309 and name N)	(segid 3A4 and resid 312 and name O)	7.62	0.07	0.07
	assign (segid 3A4 and resid 309 and name N)	(segid 3A4 and resid 313 and name CA)	7.32	0.10	0.09
	assign (segid 3A4 and resid 309 and name N)	(segid 3A4 and resid 313 and name CB)	7.16	0.14	0.14
40	assign (segid 3A4 and resid 309 and name N)	(segid 3A4 and resid 313 and name CG)	6.76	0.19	0.20
	assign (segid 3A4 and resid 309 and name N)	(segid 3A4 and resid 313 and name N)	6.14	0.09	0.08
	assign (segid 3A4 and resid 309 and name N)	(segid 3A4 and resid 365 and name CA)	6.96	0.11	0.12
	assign (segid 3A4 and resid 309 and name N)	(segid 3A4 and resid 365 and name CB)	6.51	0.15	0.15
	assign (segid 3A4 and resid 309 and name N)	(segid 3A4 and resid 365 and name O)	7.27	0.33	0.34
45	assign (segid 3A4 and resid 309 and name N)	(segid 3A4 and resid 401 and name C)	7.30	0.40	0.39
	assign (segid 3A4 and resid 309 and name N)	(segid 3A4 and resid 401 and name O)	7.29	0.40	0.39
	assign (segid 3A4 and resid 309 and name N)	(segid 3A4 and resid 402 and name CA)	7.13	0.37	0.38
	assign (segid 3A4 and resid 309 and name N)	(segid 3A4 and resid 402 and name CB)	7.34	0.36	0.36
	assign (segid 3A4 and resid 309 and name N)	(segid 3A4 and resid 402 and name N)	7.22	0.39	0.39
50	assign (segid 3A4 and resid 309 and name N)	(segid 3A4 and resid 405 and name CB)	7.10	0.35	0.34
	assign (segid 3A4 and resid 309 and name N)	(segid 3A4 and resid 309 and name CB)	3.31	0.05	0.05
	assign (segid 3A4 and resid 309 and name O)	(segid 3A4 and resid 310 and name C)	2.96	0.04	0.04
	assign (segid 3A4 and resid 309 and name O)	(segid 3A4 and resid 310 and name CA)	2.75	0.04	0.04
	assign (segid 3A4 and resid 309 and name O)	(segid 3A4 and resid 310 and name CB)	4.23	0.04	0.04
55	assign (segid 3A4 and resid 309 and name O)	(segid 3A4 and resid 310 and name N)	2.24	0.03	0.03
	assign (segid 3A4 and resid 309 and name O)	(segid 3A4 and resid 310 and name O)	3.41	0.08	0.09
	assign (segid 3A4 and resid 309 and name O)	(segid 3A4 and resid 311 and name C)	4.09	0.07	0.08
	assign (segid 3A4 and resid 309 and name O)	(segid 3A4 and resid 311 and name CA)	4.37	0.08	0.08
	assign (segid 3A4 and resid 309 and name O)	(segid 3A4 and resid 311 and name CB)	5.44	0.09	0.09
60	assign (segid 3A4 and resid 309 and name O)	(segid 3A4 and resid 311 and name CD)	7.52	0.07	0.07
	assign (segid 3A4 and resid 309 and name O)	(segid 3A4 and resid 311 and name CG)	6.63	0.07	0.06
	assign (segid 3A4 and resid 309 and name O)	(segid 3A4 and resid 311 and name N)	3.45	0.08	0.08
	assign (segid 3A4 and resid 309 and name O)	(segid 3A4 and resid 311 and name O)	5.05	0.09	0.09
	assign (segid 3A4 and resid 309 and name O)	(segid 3A4 and resid 311 and name OE1)	7.35	0.07	0.06
65	assign (segid 3A4 and resid 309 and name O)	(segid 3A4 and resid 312 and name C)	3.85	0.08	0.08
	assign (segid 3A4 and resid 309 and name O)	(segid 3A4 and resid 312 and name CA)	3.75	0.05	0.06
	assign (segid 3A4 and resid 309 and name O)	(segid 3A4 and resid 312 and name CB)	3.62	0.11	0.11
	assign (segid 3A4 and resid 309 and name O)	(segid 3A4 and resid 312 and name N)	3.27	0.07	0.08
70	assign (segid 3A4 and resid 309 and name O)	(segid 3A4 and resid 312 and name O)	5.04	0.08	0.08
	assign (segid 3A4 and resid 309 and name O)	(segid 3A4 and resid 313 and name C)	5.06	0.13	0.14
	assign (segid 3A4 and resid 309 and name O)	(segid 3A4 and resid 313 and name CA)	3.97	0.12	0.12
	assign (segid 3A4 and resid 309 and name O)	(segid 3A4 and resid 313 and name CB)	3.70	0.14	0.13
	assign (segid 3A4 and resid 309 and name O)	(segid 3A4 and resid 313 and name CG)	3.44	0.14	0.15
	assign (segid 3A4 and resid 309 and name O)	(segid 3A4 and resid 313 and name N)	3.05	0.10	0.10
75	assign (segid 3A4 and resid 309 and name O)	(segid 3A4 and resid 313 and name O)	6.20	0.15	0.14
	assign (segid 3A4 and resid 309 and name O)	(segid 3A4 and resid 314 and name C)	7.31	0.08	0.08
	assign (segid 3A4 and resid 309 and name O)	(segid 3A4 and resid 314 and name CA)	6.44	0.10	0.10
	assign (segid 3A4 and resid 309 and name O)	(segid 3A4 and resid 314 and name CB)	6.70	0.13	0.12
	assign (segid 3A4 and resid 309 and name O)	(segid 3A4 and resid 314 and name N)	5.08	0.10	0.10
80	assign (segid 3A4 and resid 309 and name O)	(segid 3A4 and resid 315 and name N)	7.01	0.07	0.07
	assign (segid 3A4 and resid 30 and name C)	(segid 3A4 and resid 30 and name O)	1.24	0.02	0.01
	assign (segid 3A4 and resid 30 and name C)	(segid 3A4 and resid 31 and name C)	3.23	0.10	0.10

	assign (segid 3A4 and resid 30 and name C) (segid 3A4 and resid 31 and name CA)	2.42	0.02	0.03
	assign (segid 3A4 and resid 30 and name C) (segid 3A4 and resid 31 and name CB)	3.60	0.09	0.09
	assign (segid 3A4 and resid 30 and name C) (segid 3A4 and resid 31 and name N)	1.32	0.02	0.01
	assign (segid 3A4 and resid 30 and name C) (segid 3A4 and resid 31 and name O)	3.59	0.21	0.21
	assign (segid 3A4 and resid 30 and name C) (segid 3A4 and resid 32 and name C)	6.50	0.09	0.08
5	assign (segid 3A4 and resid 30 and name C) (segid 3A4 and resid 32 and name CA)	5.29	0.10	0.10
	assign (segid 3A4 and resid 30 and name C) (segid 3A4 and resid 32 and name CB)	5.75	0.11	0.11
	assign (segid 3A4 and resid 30 and name C) (segid 3A4 and resid 32 and name N)	4.12	0.07	0.07
	assign (segid 3A4 and resid 30 and name C) (segid 3A4 and resid 32 and name O)	6.88	0.06	0.05
	assign (segid 3A4 and resid 30 and name C) (segid 3A4 and resid 33 and name N)	7.31	0.15	0.14
10	assign (segid 3A4 and resid 30 and name C) (segid 3A4 and resid 341 and name C)	6.77	0.25	0.24
	assign (segid 3A4 and resid 30 and name C) (segid 3A4 and resid 341 and name CA)	7.18	0.29	0.28
	assign (segid 3A4 and resid 30 and name C) (segid 3A4 and resid 341 and name CB)	6.77	0.38	0.37
	assign (segid 3A4 and resid 30 and name C) (segid 3A4 and resid 342 and name C)	4.76	0.14	0.14
	assign (segid 3A4 and resid 30 and name C) (segid 3A4 and resid 342 and name CA)	5.70	0.16	0.16
15	assign (segid 3A4 and resid 30 and name C) (segid 3A4 and resid 342 and name N)	5.81	0.20	0.20
	assign (segid 3A4 and resid 30 and name C) (segid 3A4 and resid 342 and name O)	3.65	0.15	0.15
	assign (segid 3A4 and resid 30 and name C) (segid 3A4 and resid 343 and name C)	5.98	0.13	0.14
	assign (segid 3A4 and resid 30 and name C) (segid 3A4 and resid 343 and name CA)	5.34	0.16	0.17
	assign (segid 3A4 and resid 30 and name C) (segid 3A4 and resid 343 and name CB)	6.43	0.23	0.22
20	assign (segid 3A4 and resid 30 and name C) (segid 3A4 and resid 343 and name N)	5.50	0.15	0.14
	assign (segid 3A4 and resid 30 and name C) (segid 3A4 and resid 343 and name O)	7.03	0.13	0.13
	assign (segid 3A4 and resid 30 and name C) (segid 3A4 and resid 344 and name C)	7.50	0.06	0.06
	assign (segid 3A4 and resid 30 and name C) (segid 3A4 and resid 344 and name CA)	6.67	0.12	0.12
	assign (segid 3A4 and resid 30 and name C) (segid 3A4 and resid 344 and name CB)	6.27	0.20	0.19
25	assign (segid 3A4 and resid 30 and name C) (segid 3A4 and resid 344 and name N)	5.66	0.13	0.13
	assign (segid 3A4 and resid 30 and name C) (segid 3A4 and resid 344 and name O)	7.16	0.13	0.13
	assign (segid 3A4 and resid 30 and name C) (segid 3A4 and resid 30 and name C)	1.51	0.00	0.01
	assign (segid 3A4 and resid 30 and name CA) (segid 3A4 and resid 30 and name O)	2.39	0.01	0.01
	assign (segid 3A4 and resid 30 and name CA) (segid 3A4 and resid 319 and name CA)	17.91	0.49	0.49
30	assign (segid 3A4 and resid 30 and name CA) (segid 3A4 and resid 319 and name CB)	18.18	0.52	0.52
	assign (segid 3A4 and resid 30 and name CA) (segid 3A4 and resid 31 and name C)	4.48	0.08	0.08
	assign (segid 3A4 and resid 30 and name CA) (segid 3A4 and resid 31 and name CA)	3.78	0.02	0.02
	assign (segid 3A4 and resid 30 and name CA) (segid 3A4 and resid 31 and name CB)	4.76	0.05	0.05
	assign (segid 3A4 and resid 30 and name CA) (segid 3A4 and resid 31 and name N)	2.41	0.03	0.02
35	assign (segid 3A4 and resid 30 and name CA) (segid 3A4 and resid 31 and name O)	4.53	0.21	0.22
	assign (segid 3A4 and resid 30 and name CA) (segid 3A4 and resid 322 and name CA)	9.57	0.21	0.21
	assign (segid 3A4 and resid 30 and name CA) (segid 3A4 and resid 323 and name CA)	9.81	0.23	0.24
	assign (segid 3A4 and resid 30 and name CA) (segid 3A4 and resid 323 and name CB)	10.32	0.35	0.35
	assign (segid 3A4 and resid 30 and name CA) (segid 3A4 and resid 324 and name CA)	9.35	0.33	0.32
40	assign (segid 3A4 and resid 30 and name CA) (segid 3A4 and resid 324 and name CB)	9.92	0.43	0.44
	assign (segid 3A4 and resid 30 and name CA) (segid 3A4 and resid 325 and name CA)	10.76	0.35	0.34
	assign (segid 3A4 and resid 30 and name CA) (segid 3A4 and resid 325 and name CB)	10.26	0.41	0.41
	assign (segid 3A4 and resid 30 and name CA) (segid 3A4 and resid 326 and name CA)	14.23	0.40	0.40
	assign (segid 3A4 and resid 30 and name CA) (segid 3A4 and resid 326 and name CB)	15.40	0.42	0.41
45	assign (segid 3A4 and resid 30 and name CA) (segid 3A4 and resid 327 and name CA)	15.13	0.47	0.46
	assign (segid 3A4 and resid 30 and name CA) (segid 3A4 and resid 327 and name CB)	16.46	0.50	0.51
	assign (segid 3A4 and resid 30 and name CA) (segid 3A4 and resid 328 and name CA)	14.35	0.51	0.51
	assign (segid 3A4 and resid 30 and name CA) (segid 3A4 and resid 328 and name CB)	15.18	0.50	0.51
	assign (segid 3A4 and resid 30 and name CA) (segid 3A4 and resid 329 and name CA)	14.36	0.60	0.61
50	assign (segid 3A4 and resid 30 and name CA) (segid 3A4 and resid 329 and name CB)	13.91	0.72	0.73
	assign (segid 3A4 and resid 30 and name CA) (segid 3A4 and resid 32 and name C)	7.78	0.10	0.10
	assign (segid 3A4 and resid 30 and name CA) (segid 3A4 and resid 32 and name CA)	6.50	0.10	0.09
	assign (segid 3A4 and resid 30 and name CA) (segid 3A4 and resid 32 and name CB)	6.92	0.10	0.10
	assign (segid 3A4 and resid 30 and name CA) (segid 3A4 and resid 32 and name N)	5.46	0.06	0.07
55	assign (segid 3A4 and resid 30 and name CA) (segid 3A4 and resid 330 and name CA)	14.91	0.35	0.34
	assign (segid 3A4 and resid 30 and name CA) (segid 3A4 and resid 330 and name CB)	16.22	0.32	0.33
	assign (segid 3A4 and resid 30 and name CA) (segid 3A4 and resid 331 and name CA)	13.92	0.34	0.35
	assign (segid 3A4 and resid 30 and name CA) (segid 3A4 and resid 331 and name CB)	12.64	0.36	0.37
	assign (segid 3A4 and resid 30 and name CA) (segid 3A4 and resid 332 and name CA)	16.00	0.46	0.46
60	assign (segid 3A4 and resid 30 and name CA) (segid 3A4 and resid 333 and name CA)	16.81	0.84	0.83
	assign (segid 3A4 and resid 30 and name CA) (segid 3A4 and resid 335 and name CA)	13.02	0.38	0.38
	assign (segid 3A4 and resid 30 and name CA) (segid 3A4 and resid 336 and name CA)	12.72	0.31	0.32
	assign (segid 3A4 and resid 30 and name CA) (segid 3A4 and resid 336 and name CB)	13.69	0.30	0.30
	assign (segid 3A4 and resid 30 and name CA) (segid 3A4 and resid 337 and name CA)	9.94	0.52	0.51
65	assign (segid 3A4 and resid 30 and name CA) (segid 3A4 and resid 337 and name CB)	9.53	0.62	0.63
	assign (segid 3A4 and resid 30 and name CA) (segid 3A4 and resid 338 and name CA)	10.86	0.51	0.51
	assign (segid 3A4 and resid 30 and name CA) (segid 3A4 and resid 338 and name CB)	10.79	0.62	0.61
	assign (segid 3A4 and resid 30 and name CA) (segid 3A4 and resid 339 and name CA)	12.05	0.44	0.45
	assign (segid 3A4 and resid 30 and name CA) (segid 3A4 and resid 339 and name CB)	13.49	0.41	0.42
70	assign (segid 3A4 and resid 30 and name CA) (segid 3A4 and resid 33 and name CA)	9.80	0.18	0.18
	assign (segid 3A4 and resid 30 and name CA) (segid 3A4 and resid 33 and name CB)	10.23	0.25	0.24
	assign (segid 3A4 and resid 30 and name CA) (segid 3A4 and resid 340 and name CA)	10.12	0.31	0.31
	assign (segid 3A4 and resid 30 and name CA) (segid 3A4 and resid 341 and name C)	6.14	0.36	0.35
	assign (segid 3A4 and resid 30 and name CA) (segid 3A4 and resid 341 and name CA)	6.56	0.38	0.38
75	assign (segid 3A4 and resid 30 and name CA) (segid 3A4 and resid 341 and name CB)	6.44	0.46	0.45
	assign (segid 3A4 and resid 30 and name CA) (segid 3A4 and resid 341 and name CG)	7.04	0.37	0.37
	assign (segid 3A4 and resid 30 and name CA) (segid 3A4 and resid 341 and name O)	7.01	0.36	0.37
	assign (segid 3A4 and resid 30 and name CA) (segid 3A4 and resid 342 and name C)	4.34	0.22	0.22
	assign (segid 3A4 and resid 30 and name CA) (segid 3A4 and resid 342 and name CA)	4.93	0.25	0.25
80	assign (segid 3A4 and resid 30 and name CA) (segid 3A4 and resid 342 and name N)	5.02	0.31	0.31
	assign (segid 3A4 and resid 30 and name CA) (segid 3A4 and resid 342 and name O)	3.40	0.24	0.24
	assign (segid 3A4 and resid 30 and name CA) (segid 3A4 and resid 343 and name C)	6.11	0.17	0.18

	assign (segid 3A4 and resid 30 and name CA) (segid 3A4 and resid 343 and name CA)	5.51	0.22	0.21
	assign (segid 3A4 and resid 30 and name CA) (segid 3A4 and resid 343 and name CB)	6.75	0.24	0.25
	assign (segid 3A4 and resid 30 and name CA) (segid 3A4 and resid 343 and name N)	5.28	0.21	0.21
	assign (segid 3A4 and resid 30 and name CA) (segid 3A4 and resid 344 and name O)	6.99	0.19	0.19
	assign (segid 3A4 and resid 30 and name CA) (segid 3A4 and resid 344 and name CA)	6.97	0.19	0.18
5	assign (segid 3A4 and resid 30 and name CA) (segid 3A4 and resid 344 and name CB)	6.52	0.25	0.25
	assign (segid 3A4 and resid 30 and name CA) (segid 3A4 and resid 344 and name N)	5.99	0.18	0.17
	assign (segid 3A4 and resid 30 and name CA) (segid 3A4 and resid 345 and name CA)	10.40	0.10	0.10
	assign (segid 3A4 and resid 30 and name CA) (segid 3A4 and resid 345 and name CB)	11.35	0.13	0.12
	assign (segid 3A4 and resid 30 and name CA) (segid 3A4 and resid 346 and name CA)	12.28	0.27	0.26
10	assign (segid 3A4 and resid 30 and name CA) (segid 3A4 and resid 346 and name CB)	12.05	0.38	0.39
	assign (segid 3A4 and resid 30 and name CA) (segid 3A4 and resid 347 and name CA)	15.78	0.23	0.24
	assign (segid 3A4 and resid 30 and name CA) (segid 3A4 and resid 347 and name CB)	16.39	0.25	0.26
	assign (segid 3A4 and resid 30 and name CA) (segid 3A4 and resid 348 and name CA)	17.35	0.16	0.17
	assign (segid 3A4 and resid 30 and name CA) (segid 3A4 and resid 349 and name CA)	16.45	0.36	0.36
15	assign (segid 3A4 and resid 30 and name CA) (segid 3A4 and resid 349 and name CB)	15.15	0.38	0.39
	assign (segid 3A4 and resid 30 and name CA) (segid 3A4 and resid 350 and name CA)	12.77	0.24	0.25
	assign (segid 3A4 and resid 30 and name CA) (segid 3A4 and resid 350 and name CB)	12.88	0.29	0.30
	assign (segid 3A4 and resid 30 and name CA) (segid 3A4 and resid 350 and name N)	17.83	0.69	0.69
20	assign (segid 3A4 and resid 30 and name CA) (segid 3A4 and resid 355 and name CA)	17.57	0.84	0.84
	assign (segid 3A4 and resid 30 and name CA) (segid 3A4 and resid 355 and name CB)	15.83	0.28	0.28
	assign (segid 3A4 and resid 30 and name CA) (segid 3A4 and resid 355 and name N)	18.05	0.15	0.15
	assign (segid 3A4 and resid 30 and name CA) (segid 3A4 and resid 36 and name CA)	18.57	0.24	0.25
	assign (segid 3A4 and resid 30 and name CA) (segid 3A4 and resid 37 and name CA)	19.15	0.34	0.34
	assign (segid 3A4 and resid 30 and name CA) (segid 3A4 and resid 37 and name CB)	18.79	0.95	0.96
25	assign (segid 3A4 and resid 30 and name CA) (segid 3A4 and resid 389 and name CB)	15.01	0.26	0.25
	assign (segid 3A4 and resid 30 and name CA) (segid 3A4 and resid 38 and name CA)	14.00	0.30	0.31
	assign (segid 3A4 and resid 30 and name CA) (segid 3A4 and resid 38 and name CB)	14.51	0.12	0.11
	assign (segid 3A4 and resid 30 and name CA) (segid 3A4 and resid 39 and name CA)	14.79	0.12	0.12
	assign (segid 3A4 and resid 30 and name CA) (segid 3A4 and resid 39 and name CB)	17.82	0.11	0.12
30	assign (segid 3A4 and resid 30 and name CA) (segid 3A4 and resid 40 and name CA)	19.15	0.12	0.12
	assign (segid 3A4 and resid 30 and name CA) (segid 3A4 and resid 40 and name CB)	17.02	0.39	0.39
	assign (segid 3A4 and resid 30 and name CA) (segid 3A4 and resid 41 and name CA)	16.75	0.47	0.47
	assign (segid 3A4 and resid 30 and name CA) (segid 3A4 and resid 41 and name CB)	13.91	0.35	0.34
	assign (segid 3A4 and resid 30 and name CA) (segid 3A4 and resid 42 and name CA)	12.59	0.30	0.29
35	assign (segid 3A4 and resid 30 and name CA) (segid 3A4 and resid 42 and name CB)	16.25	1.73	1.72
	assign (segid 3A4 and resid 30 and name CA) (segid 3A4 and resid 430 and name CA)	16.20	1.18	1.18
	assign (segid 3A4 and resid 30 and name CA) (segid 3A4 and resid 431 and name CA)	18.27	0.61	0.61
	assign (segid 3A4 and resid 30 and name CA) (segid 3A4 and resid 69 and name CA)	19.30	0.46	0.47
	assign (segid 3A4 and resid 30 and name CA) (segid 3A4 and resid 71 and name CB)	2.40	0.02	0.02
40	assign (segid 3A4 and resid 30 and name N) (segid 3A4 and resid 30 and name CA)	1.45	0.01	0.02
	assign (segid 3A4 and resid 30 and name N) (segid 3A4 and resid 30 and name O)	2.70	0.08	0.09
	assign (segid 3A4 and resid 30 and name N) (segid 3A4 and resid 31 and name C)	5.58	0.11	0.10
	assign (segid 3A4 and resid 30 and name N) (segid 3A4 and resid 31 and name CA)	4.75	0.11	0.10
	assign (segid 3A4 and resid 30 and name N) (segid 3A4 and resid 31 and name CB)	5.73	0.16	0.16
45	assign (segid 3A4 and resid 30 and name N) (segid 3A4 and resid 31 and name N)	3.52	0.11	0.10
	assign (segid 3A4 and resid 30 and name N) (segid 3A4 and resid 31 and name O)	5.79	0.24	0.24
	assign (segid 3A4 and resid 30 and name N) (segid 3A4 and resid 32 and name CA)	7.50	0.10	0.09
	assign (segid 3A4 and resid 30 and name N) (segid 3A4 and resid 32 and name CB)	7.72	0.15	0.15
	assign (segid 3A4 and resid 30 and name N) (segid 3A4 and resid 32 and name N)	6.41	0.07	0.08
50	assign (segid 3A4 and resid 30 and name N) (segid 3A4 and resid 341 and name C)	6.92	0.40	0.40
	assign (segid 3A4 and resid 30 and name N) (segid 3A4 and resid 341 and name CA)	7.10	0.42	0.43
	assign (segid 3A4 and resid 30 and name N) (segid 3A4 and resid 341 and name CB)	6.99	0.50	0.50
	assign (segid 3A4 and resid 30 and name N) (segid 3A4 and resid 342 and name C)	5.60	0.24	0.24
	assign (segid 3A4 and resid 30 and name N) (segid 3A4 and resid 342 and name CA)	5.96	0.29	0.30
55	assign (segid 3A4 and resid 30 and name N) (segid 3A4 and resid 342 and name N)	5.84	0.35	0.35
	assign (segid 3A4 and resid 30 and name N) (segid 3A4 and resid 342 and name O)	4.68	0.24	0.24
	assign (segid 3A4 and resid 30 and name N) (segid 3A4 and resid 343 and name C)	7.53	0.18	0.18
	assign (segid 3A4 and resid 30 and name N) (segid 3A4 and resid 343 and name CA)	6.92	0.21	0.22
	assign (segid 3A4 and resid 30 and name N) (segid 3A4 and resid 343 and name N)	6.63	0.23	0.22
60	assign (segid 3A4 and resid 30 and name N) (segid 3A4 and resid 344 and name N)	7.37	0.18	0.19
	assign (segid 3A4 and resid 30 and name O) (segid 3A4 and resid 31 and name C)	3.50	0.16	0.16
	assign (segid 3A4 and resid 30 and name O) (segid 3A4 and resid 31 and name CA)	2.77	0.07	0.07
	assign (segid 3A4 and resid 30 and name O) (segid 3A4 and resid 31 and name CB)	4.08	0.17	0.17
	assign (segid 3A4 and resid 30 and name O) (segid 3A4 and resid 31 and name N)	2.25	0.03	0.02
65	assign (segid 3A4 and resid 30 and name O) (segid 3A4 and resid 31 and name O)	4.12	0.28	0.28
	assign (segid 3A4 and resid 30 and name O) (segid 3A4 and resid 32 and name C)	6.42	0.15	0.14
	assign (segid 3A4 and resid 30 and name O) (segid 3A4 and resid 32 and name CA)	5.21	0.21	0.20
	assign (segid 3A4 and resid 30 and name O) (segid 3A4 and resid 32 and name CB)	5.40	0.25	0.25
	assign (segid 3A4 and resid 30 and name O) (segid 3A4 and resid 32 and name N)	4.04	0.16	0.15
70	assign (segid 3A4 and resid 30 and name O) (segid 3A4 and resid 32 and name O)	6.65	0.11	0.11
	assign (segid 3A4 and resid 30 and name O) (segid 3A4 and resid 33 and name N)	7.38	0.17	0.18
	assign (segid 3A4 and resid 30 and name O) (segid 3A4 and resid 342 and name C)	5.94	0.17	0.18
	assign (segid 3A4 and resid 30 and name O) (segid 3A4 and resid 342 and name CA)	6.89	0.21	0.20
	assign (segid 3A4 and resid 30 and name O) (segid 3A4 and resid 342 and name N)	6.97	0.22	0.22
75	assign (segid 3A4 and resid 30 and name O) (segid 3A4 and resid 342 and name O)	4.84	0.19	0.18
	assign (segid 3A4 and resid 30 and name O) (segid 3A4 and resid 343 and name C)	6.90	0.18	0.19
	assign (segid 3A4 and resid 30 and name O) (segid 3A4 and resid 343 and name CA)	6.36	0.17	0.18
	assign (segid 3A4 and resid 30 and name O) (segid 3A4 and resid 343 and name CB)	7.40	0.21	0.21
	assign (segid 3A4 and resid 30 and name O) (segid 3A4 and resid 343 and name N)	6.63	0.17	0.17
80	assign (segid 3A4 and resid 30 and name O) (segid 3A4 and resid 344 and name CA)	7.29	0.17	0.17
	assign (segid 3A4 and resid 30 and name O) (segid 3A4 and resid 344 and name CB)	6.73	0.18	0.17
	assign (segid 3A4 and resid 30 and name O) (segid 3A4 and resid 344 and name N)	6.41	0.18	0.18

	assign (segid 3A4 and resid 30 and name O)	(segid 3A4 and resid 344 and name O)	7.54	0.29	0.29
	assign (segid 3A4 and resid 310 and name C)	(segid 3A4 and resid 310 and name CB)	2.48	0.03	0.02
	assign (segid 3A4 and resid 310 and name C)	(segid 3A4 and resid 310 and name O)	1.23	0.01	0.01
	assign (segid 3A4 and resid 310 and name C)	(segid 3A4 and resid 311 and name C)	3.07	0.03	0.04
5	assign (segid 3A4 and resid 310 and name C)	(segid 3A4 and resid 311 and name CA)	2.44	0.02	0.02
	assign (segid 3A4 and resid 310 and name C)	(segid 3A4 and resid 311 and name CB)	3.71	0.04	0.04
	assign (segid 3A4 and resid 310 and name C)	(segid 3A4 and resid 311 and name CD)	5.46	0.04	0.04
	assign (segid 3A4 and resid 310 and name C)	(segid 3A4 and resid 311 and name CG)	4.99	0.03	0.03
	assign (segid 3A4 and resid 310 and name C)	(segid 3A4 and resid 311 and name N)	1.34	0.01	0.01
10	assign (segid 3A4 and resid 310 and name C)	(segid 3A4 and resid 311 and name O)	3.99	0.05	0.05
	assign (segid 3A4 and resid 310 and name C)	(segid 3A4 and resid 311 and name OE1)	4.93	0.06	0.07
	assign (segid 3A4 and resid 310 and name C)	(segid 3A4 and resid 312 and name C)	4.61	0.05	0.05
	assign (segid 3A4 and resid 310 and name C)	(segid 3A4 and resid 312 and name CA)	4.52	0.06	0.07
	assign (segid 3A4 and resid 310 and name C)	(segid 3A4 and resid 312 and name CB)	5.26	0.09	0.09
15	assign (segid 3A4 and resid 310 and name C)	(segid 3A4 and resid 312 and name N)	3.34	0.08	0.08
	assign (segid 3A4 and resid 310 and name C)	(segid 3A4 and resid 312 and name O)	5.69	0.05	0.05
	assign (segid 3A4 and resid 310 and name C)	(segid 3A4 and resid 313 and name C)	4.85	0.12	0.13
	assign (segid 3A4 and resid 310 and name C)	(segid 3A4 and resid 313 and name CA)	4.62	0.11	0.11
	assign (segid 3A4 and resid 310 and name C)	(segid 3A4 and resid 313 and name CB)	4.46	0.17	0.16
20	assign (segid 3A4 and resid 310 and name C)	(segid 3A4 and resid 313 and name CG)	5.12	0.14	0.13
	assign (segid 3A4 and resid 310 and name C)	(segid 3A4 and resid 313 and name N)	3.88	0.09	0.10
	assign (segid 3A4 and resid 310 and name C)	(segid 3A4 and resid 313 and name O)	6.03	0.12	0.12
	assign (segid 3A4 and resid 310 and name C)	(segid 3A4 and resid 314 and name C)	6.16	0.05	0.05
	assign (segid 3A4 and resid 310 and name C)	(segid 3A4 and resid 314 and name CA)	5.05	0.07	0.07
25	assign (segid 3A4 and resid 310 and name C)	(segid 3A4 and resid 314 and name CB)	4.68	0.08	0.07
	assign (segid 3A4 and resid 310 and name C)	(segid 3A4 and resid 314 and name CG)	6.03	0.09	0.09
	assign (segid 3A4 and resid 310 and name C)	(segid 3A4 and resid 314 and name N)	4.14	0.11	0.11
	assign (segid 3A4 and resid 310 and name C)	(segid 3A4 and resid 314 and name O)	7.32	0.05	0.05
	assign (segid 3A4 and resid 310 and name C)	(segid 3A4 and resid 315 and name CA)	7.27	0.12	0.13
30	assign (segid 3A4 and resid 310 and name C)	(segid 3A4 and resid 315 and name CB)	7.28	0.20	0.19
	assign (segid 3A4 and resid 310 and name C)	(segid 3A4 and resid 315 and name N)	6.01	0.10	0.09
	assign (segid 3A4 and resid 310 and name C)	(segid 3A4 and resid 315 and name O)	7.37	0.08	0.08
	assign (segid 3A4 and resid 310 and name C)	(segid 3A4 and resid 316 and name CA)	7.25	0.27	0.26
	assign (segid 3A4 and resid 310 and name C)	(segid 3A4 and resid 316 and name O)	7.31	0.25	0.26
35	assign (segid 3A4 and resid 310 and name CA)	(segid 3A4 and resid 310 and name C)	1.51	0.01	0.02
	assign (segid 3A4 and resid 310 and name CA)	(segid 3A4 and resid 310 and name CB)	1.51	0.01	0.01
	assign (segid 3A4 and resid 310 and name CA)	(segid 3A4 and resid 310 and name O)	2.40	0.02	0.01
	assign (segid 3A4 and resid 310 and name CA)	(segid 3A4 and resid 311 and name C)	4.44	0.04	0.03
	assign (segid 3A4 and resid 310 and name CA)	(segid 3A4 and resid 311 and name CA)	3.80	0.03	0.03
40	assign (segid 3A4 and resid 310 and name CA)	(segid 3A4 and resid 311 and name CB)	4.86	0.04	0.03
	assign (segid 3A4 and resid 310 and name CA)	(segid 3A4 and resid 311 and name CG)	6.83	0.06	0.05
	assign (segid 3A4 and resid 310 and name CA)	(segid 3A4 and resid 311 and name N)	6.27	0.04	0.04
	assign (segid 3A4 and resid 310 and name CA)	(segid 3A4 and resid 311 and name O)	2.44	0.02	0.01
45	assign (segid 3A4 and resid 310 and name CA)	(segid 3A4 and resid 311 and name OE1)	5.43	0.07	0.06
	assign (segid 3A4 and resid 310 and name CA)	(segid 3A4 and resid 312 and name C)	6.29	0.08	0.07
	assign (segid 3A4 and resid 310 and name CA)	(segid 3A4 and resid 312 and name CA)	5.56	0.06	0.05
	assign (segid 3A4 and resid 310 and name CA)	(segid 3A4 and resid 312 and name CB)	5.48	0.03	0.04
	assign (segid 3A4 and resid 310 and name CA)	(segid 3A4 and resid 312 and name N)	5.88	0.10	0.11
	assign (segid 3A4 and resid 310 and name CA)	(segid 3A4 and resid 312 and name O)	4.40	0.06	0.05
50	assign (segid 3A4 and resid 310 and name CA)	(segid 3A4 and resid 312 and name O)	6.70	0.07	0.06
	assign (segid 3A4 and resid 310 and name CA)	(segid 3A4 and resid 313 and name C)	5.74	0.15	0.16
	assign (segid 3A4 and resid 310 and name CA)	(segid 3A4 and resid 313 and name CA)	5.25	0.13	0.14
	assign (segid 3A4 and resid 310 and name CA)	(segid 3A4 and resid 313 and name CB)	4.68	0.20	0.20
	assign (segid 3A4 and resid 310 and name CA)	(segid 3A4 and resid 313 and name CG)	4.98	0.19	0.19
55	assign (segid 3A4 and resid 310 and name CA)	(segid 3A4 and resid 313 and name N)	4.64	0.09	0.10
	assign (segid 3A4 and resid 310 and name CA)	(segid 3A4 and resid 313 and name O)	6.88	0.17	0.16
	assign (segid 3A4 and resid 310 and name CA)	(segid 3A4 and resid 314 and name C)	7.46	0.07	0.07
	assign (segid 3A4 and resid 310 and name CA)	(segid 3A4 and resid 314 and name CA)	6.26	0.08	0.09
	assign (segid 3A4 and resid 310 and name CA)	(segid 3A4 and resid 314 and name CB)	5.98	0.09	0.09
60	assign (segid 3A4 and resid 310 and name CA)	(segid 3A4 and resid 314 and name CG)	7.30	0.10	0.10
	assign (segid 3A4 and resid 310 and name CA)	(segid 3A4 and resid 314 and name N)	5.26	0.13	0.13
	assign (segid 3A4 and resid 310 and name CA)	(segid 3A4 and resid 315 and name CA)	8.69	0.12	0.11
	assign (segid 3A4 and resid 310 and name CA)	(segid 3A4 and resid 315 and name CB)	8.71	0.19	0.18
	assign (segid 3A4 and resid 310 and name CA)	(segid 3A4 and resid 315 and name N)	7.40	0.09	0.10
65	assign (segid 3A4 and resid 310 and name CA)	(segid 3A4 and resid 316 and name CA)	10.10	0.16	0.16
	assign (segid 3A4 and resid 310 and name CA)	(segid 3A4 and resid 317 and name CA)	10.35	0.51	0.50
	assign (segid 3A4 and resid 310 and name CA)	(segid 3A4 and resid 318 and name CA)	12.60	0.50	0.49
	assign (segid 3A4 and resid 310 and name CA)	(segid 3A4 and resid 318 and name CB)	12.28	0.54	0.53
	assign (segid 3A4 and resid 310 and name CA)	(segid 3A4 and resid 319 and name CA)	14.58	0.45	0.45
70	assign (segid 3A4 and resid 310 and name CA)	(segid 3A4 and resid 319 and name CB)	14.41	0.42	0.42
	assign (segid 3A4 and resid 310 and name CA)	(segid 3A4 and resid 319 and name N)	17.93	0.36	0.36
	assign (segid 3A4 and resid 310 and name CA)	(segid 3A4 and resid 319 and name O)	18.62	0.33	0.32
	assign (segid 3A4 and resid 310 and name CA)	(segid 3A4 and resid 319 and name O)	14.28	0.37	0.37
	assign (segid 3A4 and resid 310 and name CA)	(segid 3A4 and resid 319 and name O)	13.63	0.41	0.42
75	assign (segid 3A4 and resid 310 and name CA)	(segid 3A4 and resid 319 and name O)	13.67	0.43	0.43
	assign (segid 3A4 and resid 310 and name CA)	(segid 3A4 and resid 319 and name O)	15.92	0.40	0.41
	assign (segid 3A4 and resid 310 and name CA)	(segid 3A4 and resid 319 and name O)	17.34	0.36	0.36
	assign (segid 3A4 and resid 310 and name CA)	(segid 3A4 and resid 319 and name O)	14.39	0.33	0.33
	assign (segid 3A4 and resid 310 and name CA)	(segid 3A4 and resid 319 and name O)	14.17	0.45	0.45
80	assign (segid 3A4 and resid 310 and name CA)	(segid 3A4 and resid 319 and name O)	11.11	0.23	0.23
	assign (segid 3A4 and resid 310 and name CA)	(segid 3A4 and resid 319 and name O)	13.52	0.30	0.29
	assign (segid 3A4 and resid 310 and name CA)	(segid 3A4 and resid 319 and name O)	14.19	0.29	0.29
	assign (segid 3A4 and resid 310 and name CA)	(segid 3A4 and resid 319 and name O)	15.83	0.36	0.36

	assign (segid 3A4 and resid 310 and name CA) (segid 3A4 and resid 353 and name CB)	15.94	0.41	0.42
	assign (segid 3A4 and resid 310 and name CA) (segid 3A4 and resid 354 and name CA)	17.24	0.38	0.38
	assign (segid 3A4 and resid 310 and name CA) (segid 3A4 and resid 354 and name CB)	18.52	0.41	0.42
	assign (segid 3A4 and resid 310 and name CA) (segid 3A4 and resid 355 and name CA)	18.32	0.48	0.47
5	assign (segid 3A4 and resid 310 and name CA) (segid 3A4 and resid 355 and name CB)	19.21	0.48	0.47
	assign (segid 3A4 and resid 310 and name CA) (segid 3A4 and resid 356 and name CA)	14.89	0.49	0.50
	assign (segid 3A4 and resid 310 and name CA) (segid 3A4 and resid 356 and name CB)	14.23	0.47	0.47
	assign (segid 3A4 and resid 310 and name CA) (segid 3A4 and resid 357 and name CA)	12.98	0.39	0.40
	assign (segid 3A4 and resid 310 and name CA) (segid 3A4 and resid 357 and name CB)	11.88	0.46	0.46
10	assign (segid 3A4 and resid 310 and name CA) (segid 3A4 and resid 358 and name CA)	15.87	0.85	0.85
	assign (segid 3A4 and resid 310 and name CA) (segid 3A4 and resid 358 and name CB)	16.47	1.18	1.18
	assign (segid 3A4 and resid 310 and name CA) (segid 3A4 and resid 359 and name CA)	15.80	0.22	0.22
	assign (segid 3A4 and resid 310 and name CA) (segid 3A4 and resid 359 and name CB)	15.96	0.23	0.24
	assign (segid 3A4 and resid 310 and name CA) (segid 3A4 and resid 360 and name CA)	13.43	0.18	0.18
15	assign (segid 3A4 and resid 310 and name CA) (segid 3A4 and resid 360 and name CB)	14.04	0.25	0.25
	assign (segid 3A4 and resid 310 and name CA) (segid 3A4 and resid 361 and name CA)	14.48	0.19	0.18
	assign (segid 3A4 and resid 310 and name CA) (segid 3A4 and resid 361 and name CB)	15.92	0.21	0.21
	assign (segid 3A4 and resid 310 and name CA) (segid 3A4 and resid 362 and name CA)	13.51	0.13	0.13
	assign (segid 3A4 and resid 310 and name CA) (segid 3A4 and resid 362 and name CB)	14.17	0.15	0.15
20	assign (segid 3A4 and resid 310 and name CA) (segid 3A4 and resid 363 and name CA)	10.65	0.11	0.11
	assign (segid 3A4 and resid 310 and name CA) (segid 3A4 and resid 363 and name CB)	10.80	0.18	0.19
	assign (segid 3A4 and resid 310 and name CA) (segid 3A4 and resid 364 and name CA)	10.11	0.07	0.08
	assign (segid 3A4 and resid 310 and name CA) (segid 3A4 and resid 364 and name CB)	11.04	0.06	0.06
	assign (segid 3A4 and resid 310 and name CA) (segid 3A4 and resid 365 and name CA)	7.86	0.27	0.27
25	assign (segid 3A4 and resid 310 and name CA) (segid 3A4 and resid 365 and name CB)	8.22	0.34	0.34
	assign (segid 3A4 and resid 310 and name CA) (segid 3A4 and resid 381 and name CA)	8.44	0.36	0.35
	assign (segid 3A4 and resid 310 and name CA) (segid 3A4 and resid 382 and name CA)	10.52	0.13	0.13
	assign (segid 3A4 and resid 310 and name CA) (segid 3A4 and resid 382 and name CB)	11.96	0.16	0.17
	assign (segid 3A4 and resid 310 and name CA) (segid 3A4 and resid 383 and name CA)	9.10	0.25	0.26
30	assign (segid 3A4 and resid 310 and name CA) (segid 3A4 and resid 384 and name CA)	10.73	0.48	0.48
	assign (segid 3A4 and resid 310 and name CA) (segid 3A4 and resid 384 and name CB)	10.25	0.57	0.57
	assign (segid 3A4 and resid 310 and name CA) (segid 3A4 and resid 385 and name CA)	13.65	0.41	0.40
	assign (segid 3A4 and resid 310 and name CA) (segid 3A4 and resid 386 and name CA)	15.41	0.45	0.46
	assign (segid 3A4 and resid 310 and name CA) (segid 3A4 and resid 387 and name CA)	18.60	0.40	0.40
35	assign (segid 3A4 and resid 310 and name CA) (segid 3A4 and resid 390 and name CA)	15.84	0.56	0.55
	assign (segid 3A4 and resid 310 and name CA) (segid 3A4 and resid 390 and name CB)	15.38	0.50	0.49
	assign (segid 3A4 and resid 310 and name CA) (segid 3A4 and resid 391 and name CA)	14.65	0.59	0.60
	assign (segid 3A4 and resid 310 and name CA) (segid 3A4 and resid 391 and name CB)	13.37	0.60	0.59
	assign (segid 3A4 and resid 310 and name CA) (segid 3A4 and resid 392 and name CA)	16.67	0.60	0.60
40	assign (segid 3A4 and resid 310 and name CA) (segid 3A4 and resid 392 and name CB)	18.14	0.61	0.60
	assign (segid 3A4 and resid 310 and name CA) (segid 3A4 and resid 393 and name CA)	14.91	0.57	0.57
	assign (segid 3A4 and resid 310 and name CA) (segid 3A4 and resid 394 and name CA)	11.39	0.61	0.62
	assign (segid 3A4 and resid 310 and name CA) (segid 3A4 and resid 394 and name CB)	11.14	0.70	0.71
	assign (segid 3A4 and resid 310 and name CA) (segid 3A4 and resid 395 and name CA)	12.19	0.63	0.62
45	assign (segid 3A4 and resid 310 and name CA) (segid 3A4 and resid 396 and name CA)	13.76	0.49	0.49
	assign (segid 3A4 and resid 310 and name CA) (segid 3A4 and resid 396 and name CB)	15.01	0.51	0.52
	assign (segid 3A4 and resid 310 and name CA) (segid 3A4 and resid 397 and name CA)	11.14	0.53	0.54
	assign (segid 3A4 and resid 310 and name CA) (segid 3A4 and resid 397 and name CB)	10.71	0.59	0.59
	assign (segid 3A4 and resid 310 and name CA) (segid 3A4 and resid 398 and name CA)	8.51	0.45	0.46
50	assign (segid 3A4 and resid 310 and name CA) (segid 3A4 and resid 398 and name CB)	8.04	0.54	0.53
	assign (segid 3A4 and resid 310 and name CA) (segid 3A4 and resid 399 and name CA)	11.59	0.37	0.38
	assign (segid 3A4 and resid 310 and name CA) (segid 3A4 and resid 399 and name CB)	12.89	0.40	0.40
	assign (segid 3A4 and resid 310 and name CA) (segid 3A4 and resid 400 and name CA)	12.79	0.32	0.31
	assign (segid 3A4 and resid 310 and name CA) (segid 3A4 and resid 400 and name CB)	13.29	0.26	0.27
55	assign (segid 3A4 and resid 310 and name CA) (segid 3A4 and resid 401 and name CA)	9.85	0.30	0.31
	assign (segid 3A4 and resid 310 and name CA) (segid 3A4 and resid 402 and name CA)	9.83	0.31	0.31
	assign (segid 3A4 and resid 310 and name CA) (segid 3A4 and resid 402 and name CB)	9.65	0.31	0.31
	assign (segid 3A4 and resid 310 and name CA) (segid 3A4 and resid 403 and name CA)	13.61	0.30	0.30
	assign (segid 3A4 and resid 310 and name CA) (segid 3A4 and resid 403 and name CB)	14.50	0.28	0.28
60	assign (segid 3A4 and resid 310 and name CA) (segid 3A4 and resid 404 and name CA)	14.13	0.34	0.35
	assign (segid 3A4 and resid 310 and name CA) (segid 3A4 and resid 404 and name CB)	13.82	0.43	0.43
	assign (segid 3A4 and resid 310 and name CA) (segid 3A4 and resid 405 and name CA)	12.33	0.27	0.27
	assign (segid 3A4 and resid 310 and name CA) (segid 3A4 and resid 405 and name CB)	10.89	0.26	0.26
65	assign (segid 3A4 and resid 310 and name CA) (segid 3A4 and resid 406 and name CA)	13.94	0.46	0.45
	assign (segid 3A4 and resid 310 and name CA) (segid 3A4 and resid 407 and name CA)	17.20	0.35	0.35
	assign (segid 3A4 and resid 310 and name CA) (segid 3A4 and resid 407 and name CB)	17.68	0.34	0.35
	assign (segid 3A4 and resid 310 and name CA) (segid 3A4 and resid 408 and name CA)	17.36	0.20	0.20
	assign (segid 3A4 and resid 310 and name CA) (segid 3A4 and resid 408 and name CB)	16.54	0.20	0.21
	assign (segid 3A4 and resid 310 and name CA) (segid 3A4 and resid 409 and name CA)	17.02	0.52	0.52
70	assign (segid 3A4 and resid 310 and name CA) (segid 3A4 and resid 409 and name CB)	15.87	0.64	0.63
	assign (segid 3A4 and resid 310 and name CA) (segid 3A4 and resid 410 and name CA)	19.40	0.41	0.41
	assign (segid 3A4 and resid 310 and name CA) (segid 3A4 and resid 433 and name CA)	16.86	0.60	0.61
	assign (segid 3A4 and resid 310 and name CA) (segid 3A4 and resid 434 and name CA)	16.81	0.94	0.94
	assign (segid 3A4 and resid 310 and name CA) (segid 3A4 and resid 435 and name CA)	18.05	0.94	0.95
75	assign (segid 3A4 and resid 310 and name CB) (segid 3A4 and resid 311 and name C)	5.45	0.06	0.05
	assign (segid 3A4 and resid 310 and name CB) (segid 3A4 and resid 311 and name CA)	4.46	0.04	0.04
	assign (segid 3A4 and resid 310 and name CB) (segid 3A4 and resid 311 and name CB)	5.28	0.04	0.04
	assign (segid 3A4 and resid 310 and name CB) (segid 3A4 and resid 311 and name CD)	7.11	0.07	0.08
	assign (segid 3A4 and resid 310 and name CB) (segid 3A4 and resid 311 and name CG)	6.72	0.05	0.05
80	assign (segid 3A4 and resid 310 and name CB) (segid 3A4 and resid 311 and name N)	3.13	0.05	0.05
	assign (segid 3A4 and resid 310 and name CB) (segid 3A4 and resid 311 and name O)	6.40	0.07	0.07
	assign (segid 3A4 and resid 310 and name CB) (segid 3A4 and resid 311 and name OE1)	6.42	0.10	0.10
	assign (segid 3A4 and resid 310 and name CB) (segid 3A4 and resid 312 and name C)	6.95	0.06	0.06

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5	assign	(segid 3A4 and resid 310 and name CB)	(segid 3A4 and resid 398 and name CB)	8.36	0.55	0.55
	assign	(segid 3A4 and resid 310 and name CB)	(segid 3A4 and resid 399 and name CB)	12.00	0.38	0.38
	assign	(segid 3A4 and resid 310 and name CB)	(segid 3A4 and resid 399 and name CB)	13.23	0.41	0.42
	assign	(segid 3A4 and resid 310 and name CB)	(segid 3A4 and resid 400 and name CB)	13.58	0.31	0.30
	assign	(segid 3A4 and resid 310 and name CB)	(segid 3A4 and resid 400 and name CB)	14.17	0.26	0.26
10	assign	(segid 3A4 and resid 310 and name CB)	(segid 3A4 and resid 401 and name CA)	10.84	0.27	0.27
	assign	(segid 3A4 and resid 310 and name CB)	(segid 3A4 and resid 402 and name CA)	10.40	0.31	0.31
	assign	(segid 3A4 and resid 310 and name CB)	(segid 3A4 and resid 402 and name CB)	10.02	0.31	0.31
	assign	(segid 3A4 and resid 310 and name CB)	(segid 3A4 and resid 403 and name CA)	14.20	0.30	0.29
	assign	(segid 3A4 and resid 310 and name CB)	(segid 3A4 and resid 403 and name CB)	15.08	0.29	0.28
15	assign	(segid 3A4 and resid 310 and name CB)	(segid 3A4 and resid 404 and name CA)	15.04	0.33	0.33
	assign	(segid 3A4 and resid 310 and name CB)	(segid 3A4 and resid 404 and name CB)	14.83	0.40	0.40
	assign	(segid 3A4 and resid 310 and name CB)	(segid 3A4 and resid 405 and name CA)	13.20	0.33	0.32
	assign	(segid 3A4 and resid 310 and name CB)	(segid 3A4 and resid 405 and name CB)	11.78	0.29	0.28
	assign	(segid 3A4 and resid 310 and name CB)	(segid 3A4 and resid 406 and name CA)	14.47	0.50	0.49
20	assign	(segid 3A4 and resid 310 and name CB)	(segid 3A4 and resid 407 and name CA)	17.86	0.40	0.41
	assign	(segid 3A4 and resid 310 and name CB)	(segid 3A4 and resid 407 and name CB)	18.38	0.39	0.39
	assign	(segid 3A4 and resid 310 and name CB)	(segid 3A4 and resid 408 and name CA)	18.24	0.28	0.28
	assign	(segid 3A4 and resid 310 and name CB)	(segid 3A4 and resid 408 and name CB)	17.51	0.29	0.30
	assign	(segid 3A4 and resid 310 and name CB)	(segid 3A4 and resid 409 and name CA)	17.75	0.53	0.52
25	assign	(segid 3A4 and resid 310 and name CB)	(segid 3A4 and resid 409 and name CB)	16.55	0.64	0.63
	assign	(segid 3A4 and resid 310 and name CB)	(segid 3A4 and resid 433 and name CA)	18.21	0.55	0.55
	assign	(segid 3A4 and resid 310 and name CB)	(segid 3A4 and resid 434 and name CA)	18.25	0.93	0.93
	assign	(segid 3A4 and resid 310 and name N)	(segid 3A4 and resid 310 and name C)	2.47	0.02	0.02
	assign	(segid 3A4 and resid 310 and name N)	(segid 3A4 and resid 310 and name CA)	1.47	0.02	0.01
30	assign	(segid 3A4 and resid 310 and name N)	(segid 3A4 and resid 310 and name CB)	2.44	0.02	0.03
	assign	(segid 3A4 and resid 310 and name N)	(segid 3A4 and resid 310 and name O)	3.50	0.04	0.04
	assign	(segid 3A4 and resid 310 and name N)	(segid 3A4 and resid 311 and name C)	4.71	0.02	0.02
	assign	(segid 3A4 and resid 310 and name N)	(segid 3A4 and resid 311 and name CA)	4.22	0.03	0.03
	assign	(segid 3A4 and resid 310 and name N)	(segid 3A4 and resid 311 and name CB)	5.00	0.02	0.03
35	assign	(segid 3A4 and resid 310 and name N)	(segid 3A4 and resid 311 and name CD)	7.31	0.05	0.04
	assign	(segid 3A4 and resid 310 and name N)	(segid 3A4 and resid 311 and name CG)	6.47	0.03	0.02
	assign	(segid 3A4 and resid 310 and name N)	(segid 3A4 and resid 311 and name N)	2.83	0.03	0.03
	assign	(segid 3A4 and resid 310 and name N)	(segid 3A4 and resid 311 and name O)	5.85	0.03	0.03
	assign	(segid 3A4 and resid 310 and name N)	(segid 3A4 and resid 311 and name OE1)	6.98	0.06	0.07
40	assign	(segid 3A4 and resid 310 and name N)	(segid 3A4 and resid 312 and name C)	5.67	0.04	0.04
	assign	(segid 3A4 and resid 310 and name N)	(segid 3A4 and resid 312 and name CA)	5.32	0.07	0.07
	assign	(segid 3A4 and resid 310 and name N)	(segid 3A4 and resid 312 and name CB)	5.36	0.13	0.14
	assign	(segid 3A4 and resid 310 and name N)	(segid 3A4 and resid 312 and name N)	4.31	0.08	0.07
	assign	(segid 3A4 and resid 310 and name N)	(segid 3A4 and resid 312 and name O)	6.88	0.04	0.04
45	assign	(segid 3A4 and resid 310 and name N)	(segid 3A4 and resid 313 and name C)	6.51	0.12	0.12
	assign	(segid 3A4 and resid 310 and name N)	(segid 3A4 and resid 313 and name CA)	5.74	0.11	0.12
	assign	(segid 3A4 and resid 310 and name N)	(segid 3A4 and resid 313 and name CB)	5.25	0.17	0.17
	assign	(segid 3A4 and resid 310 and name N)	(segid 3A4 and resid 313 and name CG)	5.17	0.17	0.18
	assign	(segid 3A4 and resid 310 and name N)	(segid 3A4 and resid 313 and name N)	4.90	0.09	0.08
50	assign	(segid 3A4 and resid 310 and name N)	(segid 3A4 and resid 313 and name O)	7.68	0.14	0.14
	assign	(segid 3A4 and resid 310 and name N)	(segid 3A4 and resid 314 and name CA)	7.30	0.06	0.05
	assign	(segid 3A4 and resid 310 and name N)	(segid 3A4 and resid 314 and name CB)	7.10	0.08	0.09
	assign	(segid 3A4 and resid 310 and name N)	(segid 3A4 and resid 314 and name N)	6.16	0.08	0.08
	assign	(segid 3A4 and resid 310 and name N)	(segid 3A4 and resid 365 and name O)	7.50	0.18	0.17
55	assign	(segid				

	assign (segid 3A4 and resid 311 and name C) (segid 3A4 and resid 311 and name CD)	3.73	0.09	0.09
	assign (segid 3A4 and resid 311 and name C) (segid 3A4 and resid 311 and name CG)	3.02	0.06	0.06
	assign (segid 3A4 and resid 311 and name C) (segid 3A4 and resid 311 and name O)	1.25	0.02	0.02
	assign (segid 3A4 and resid 311 and name C) (segid 3A4 and resid 311 and name OE1)	3.83	0.09	0.10
5	assign (segid 3A4 and resid 311 and name C) (segid 3A4 and resid 312 and name C)	3.04	0.04	0.04
	assign (segid 3A4 and resid 311 and name C) (segid 3A4 and resid 312 and name CA)	2.44	0.03	0.04
	assign (segid 3A4 and resid 311 and name C) (segid 3A4 and resid 312 and name CB)	3.72	0.03	0.03
	assign (segid 3A4 and resid 311 and name C) (segid 3A4 and resid 312 and name N)	1.34	0.01	0.01
	assign (segid 3A4 and resid 311 and name C) (segid 3A4 and resid 312 and name O)	3.87	0.06	0.05
10	assign (segid 3A4 and resid 311 and name C) (segid 3A4 and resid 313 and name C)	4.51	0.08	0.08
	assign (segid 3A4 and resid 311 and name C) (segid 3A4 and resid 313 and name CA)	4.49	0.04	0.05
	assign (segid 3A4 and resid 311 and name C) (segid 3A4 and resid 313 and name CB)	5.29	0.06	0.05
	assign (segid 3A4 and resid 311 and name C) (segid 3A4 and resid 313 and name CG)	6.09	0.13	0.13
	assign (segid 3A4 and resid 311 and name C) (segid 3A4 and resid 313 and name N)	3.32	0.04	0.04
15	assign (segid 3A4 and resid 311 and name C) (segid 3A4 and resid 313 and name O)	5.63	0.11	0.11
	assign (segid 3A4 and resid 311 and name C) (segid 3A4 and resid 314 and name C)	4.81	0.05	0.05
	assign (segid 3A4 and resid 311 and name C) (segid 3A4 and resid 314 and name CA)	4.45	0.02	0.03
	assign (segid 3A4 and resid 311 and name C) (segid 3A4 and resid 314 and name CB)	4.25	0.06	0.05
	assign (segid 3A4 and resid 311 and name C) (segid 3A4 and resid 314 and name CG)	5.54	0.09	0.09
20	assign (segid 3A4 and resid 311 and name C) (segid 3A4 and resid 314 and name N)	3.71	0.05	0.06
	assign (segid 3A4 and resid 311 and name C) (segid 3A4 and resid 314 and name O)	6.03	0.06	0.05
	assign (segid 3A4 and resid 311 and name C) (segid 3A4 and resid 315 and name C)	5.91	0.14	0.14
	assign (segid 3A4 and resid 311 and name C) (segid 3A4 and resid 315 and name CA)	4.93	0.16	0.17
	assign (segid 3A4 and resid 311 and name C) (segid 3A4 and resid 315 and name CB)	4.50	0.22	0.23
25	assign (segid 3A4 and resid 311 and name C) (segid 3A4 and resid 315 and name N)	4.04	0.11	0.11
	assign (segid 3A4 and resid 311 and name C) (segid 3A4 and resid 315 and name O)	7.09	0.14	0.15
	assign (segid 3A4 and resid 311 and name C) (segid 3A4 and resid 316 and name C)	7.55	0.19	0.20
	assign (segid 3A4 and resid 311 and name C) (segid 3A4 and resid 316 and name CA)	7.01	0.17	0.17
	assign (segid 3A4 and resid 311 and name C) (segid 3A4 and resid 316 and name N)	5.74	0.16	0.16
30	assign (segid 3A4 and resid 311 and name C) (segid 3A4 and resid 362 and name O)	7.45	0.13	0.12
	assign (segid 3A4 and resid 311 and name C) (segid 3A4 and resid 363 and name C)	7.04	0.04	0.05
	assign (segid 3A4 and resid 311 and name C) (segid 3A4 and resid 363 and name CA)	6.64	0.07	0.07
	assign (segid 3A4 and resid 311 and name C) (segid 3A4 and resid 363 and name CB)	6.68	0.15	0.15
	assign (segid 3A4 and resid 311 and name C) (segid 3A4 and resid 363 and name CG)	5.76	0.15	0.14
35	assign (segid 3A4 and resid 311 and name C) (segid 3A4 and resid 363 and name N)	7.84	0.10	0.10
	assign (segid 3A4 and resid 311 and name C) (segid 3A4 and resid 364 and name C)	6.64	0.11	0.11
	assign (segid 3A4 and resid 311 and name C) (segid 3A4 and resid 364 and name CA)	7.32	0.09	0.09
	assign (segid 3A4 and resid 311 and name C) (segid 3A4 and resid 364 and name N)	6.56	0.09	0.09
	assign (segid 3A4 and resid 311 and name C) (segid 3A4 and resid 364 and name O)	6.36	0.19	0.19
40	assign (segid 3A4 and resid 311 and name C) (segid 3A4 and resid 365 and name C)	7.53	0.14	0.14
	assign (segid 3A4 and resid 311 and name C) (segid 3A4 and resid 365 and name CA)	6.57	0.14	0.13
	assign (segid 3A4 and resid 311 and name C) (segid 3A4 and resid 365 and name CB)	7.13	0.13	0.12
	assign (segid 3A4 and resid 311 and name C) (segid 3A4 and resid 365 and name N)	6.76	0.10	0.11
	assign (segid 3A4 and resid 311 and name C) (segid 3A4 and resid 365 and name O)	7.58	0.16	0.16
45	assign (segid 3A4 and resid 311 and name CA) (segid 3A4 and resid 311 and name C)	1.51	0.02	0.03
	assign (segid 3A4 and resid 311 and name CA) (segid 3A4 and resid 311 and name CB)	1.55	0.02	0.01
	assign (segid 3A4 and resid 311 and name CA) (segid 3A4 and resid 311 and name CD)	3.20	0.03	0.03
	assign (segid 3A4 and resid 311 and name CA) (segid 3A4 and resid 311 and name CG)	2.58	0.01	0.02
	assign (segid 3A4 and resid 311 and name CA) (segid 3A4 and resid 311 and name O)	2.41	0.02	0.01
50	assign (segid 3A4 and resid 311 and name CA) (segid 3A4 and resid 311 and name OE1)	3.04	0.07	0.06
	assign (segid 3A4 and resid 311 and name CA) (segid 3A4 and resid 312 and name C)	4.41	0.03	0.03
	assign (segid 3A4 and resid 311 and name CA) (segid 3A4 and resid 312 and name CA)	3.83	0.04	0.03
	assign (segid 3A4 and resid 311 and name CA) (segid 3A4 and resid 312 and name CB)	4.90	0.02	0.02
	assign (segid 3A4 and resid 311 and name CA) (segid 3A4 and resid 312 and name N)	2.47	0.03	0.03
55	assign (segid 3A4 and resid 311 and name CA) (segid 3A4 and resid 312 and name O)	5.31	0.05	0.04
	assign (segid 3A4 and resid 311 and name CA) (segid 3A4 and resid 313 and name C)	5.38	0.12	0.11
	assign (segid 3A4 and resid 311 and name CA) (segid 3A4 and resid 313 and name CA)	5.43	0.08	0.08
	assign (segid 3A4 and resid 311 and name CA) (segid 3A4 and resid 313 and name CB)	5.91	0.11	0.11
	assign (segid 3A4 and resid 311 and name CA) (segid 3A4 and resid 313 and name CG)	6.72	0.13	0.13
60	assign (segid 3A4 and resid 311 and name CA) (segid 3A4 and resid 313 and name N)	4.38	0.07	0.07
	assign (segid 3A4 and resid 311 and name CA) (segid 3A4 and resid 313 and name O)	6.51	0.13	0.13
	assign (segid 3A4 and resid 311 and name CA) (segid 3A4 and resid 314 and name C)	5.57	0.04	0.05
	assign (segid 3A4 and resid 311 and name CA) (segid 3A4 and resid 314 and name CA)	4.95	0.07	0.07
	assign (segid 3A4 and resid 311 and name CA) (segid 3A4 and resid 314 and name CB)	4.32	0.07	0.06
65	assign (segid 3A4 and resid 311 and name CA) (segid 3A4 and resid 314 and name CG)	5.50	0.07	0.07
	assign (segid 3A4 and resid 311 and name CA) (segid 3A4 and resid 314 and name N)	4.39	0.11	0.11
	assign (segid 3A4 and resid 311 and name CA) (segid 3A4 and resid 314 and name O)	6.79	0.06	0.06
	assign (segid 3A4 and resid 311 and name CA) (segid 3A4 and resid 315 and name C)	7.12	0.12	0.13
	assign (segid 3A4 and resid 311 and name CA) (segid 3A4 and resid 315 and name CA)	5.99	0.17	0.16
70	assign (segid 3A4 and resid 311 and name CA) (segid 3A4 and resid 315 and name CB)	5.60	0.24	0.23
	assign (segid 3A4 and resid 311 and name CA) (segid 3A4 and resid 315 and name N)	5.00	0.10	0.09
	assign (segid 3A4 and resid 311 and name CA) (segid 3A4 and resid 316 and name CA)	8.39	0.14	0.14
	assign (segid 3A4 and resid 311 and name CA) (segid 3A4 and resid 316 and name N)	7.08	0.13	0.14
	assign (segid 3A4 and resid 311 and name CA) (segid 3A4 and resid 317 and name CA)	9.71	0.20	0.21
75	assign (segid 3A4 and resid 311 and name CA) (segid 3A4 and resid 318 and name CA)	12.47	0.33	0.33
	assign (segid 3A4 and resid 311 and name CA) (segid 3A4 and resid 318 and name CB)	12.41	0.35	0.35
	assign (segid 3A4 and resid 311 and name CA) (segid 3A4 and resid 319 and name CA)	14.92	0.33	0.33
	assign (segid 3A4 and resid 311 and name CA) (segid 3A4 and resid 319 and name CB)	15.12	0.27	0.26
	assign (segid 3A4 and resid 311 and name CA) (segid 3A4 and resid 346 and name CA)	17.43	0.32	0.31
80	assign (segid 3A4 and resid 311 and name CA) (segid 3A4 and resid 346 and name CB)	17.83	0.25	0.26
	assign (segid 3A4 and resid 311 and name CA) (segid 3A4 and resid 347 and name CA)	14.09	0.40	0.40
	assign (segid 3A4 and resid 311 and name CA) (segid 3A4 and resid 347 and name CB)	13.77	0.47	0.47
	assign (segid 3A4 and resid 311 and name CA) (segid 3A4 and resid 348 and name CA)	12.57	0.40	0.39

	assign (segid 3A4 and resid 311 and name CA)	(segid 3A4 and resid 349 and name CA)	14.47	0.34	0.35
	assign (segid 3A4 and resid 311 and name CA)	(segid 3A4 and resid 349 and name CB)	15.96	0.33	0.33
	assign (segid 3A4 and resid 311 and name CA)	(segid 3A4 and resid 350 and name CA)	13.46	0.21	0.22
	assign (segid 3A4 and resid 311 and name CA)	(segid 3A4 and resid 350 and name CB)	13.65	0.33	0.33
5	assign (segid 3A4 and resid 311 and name CA)	(segid 3A4 and resid 351 and name CA)	9.79	0.16	0.15
	assign (segid 3A4 and resid 311 and name CA)	(segid 3A4 and resid 352 and name CA)	11.26	0.26	0.25
	assign (segid 3A4 and resid 311 and name CA)	(segid 3A4 and resid 352 and name CB)	11.80	0.22	0.22
	assign (segid 3A4 and resid 311 and name CA)	(segid 3A4 and resid 353 and name CA)	13.93	0.36	0.35
	assign (segid 3A4 and resid 311 and name CA)	(segid 3A4 and resid 353 and name CB)	14.37	0.40	0.40
10	assign (segid 3A4 and resid 311 and name CA)	(segid 3A4 and resid 354 and name CA)	14.89	0.43	0.43
	assign (segid 3A4 and resid 311 and name CA)	(segid 3A4 and resid 354 and name CB)	16.02	0.48	0.47
	assign (segid 3A4 and resid 311 and name CA)	(segid 3A4 and resid 355 and name CA)	16.56	0.51	0.50
	assign (segid 3A4 and resid 311 and name CA)	(segid 3A4 and resid 355 and name CB)	17.62	0.46	0.46
	assign (segid 3A4 and resid 311 and name CA)	(segid 3A4 and resid 356 and name CA)	13.54	0.48	0.49
15	assign (segid 3A4 and resid 311 and name CA)	(segid 3A4 and resid 356 and name CB)	13.11	0.46	0.46
	assign (segid 3A4 and resid 311 and name CA)	(segid 3A4 and resid 357 and name CA)	10.89	0.45	0.45
	assign (segid 3A4 and resid 311 and name CA)	(segid 3A4 and resid 357 and name CB)	9.67	0.49	0.50
	assign (segid 3A4 and resid 311 and name CA)	(segid 3A4 and resid 358 and name CA)	13.13	0.71	0.72
	assign (segid 3A4 and resid 311 and name CA)	(segid 3A4 and resid 358 and name CB)	13.78	1.03	1.03
20	assign (segid 3A4 and resid 311 and name CA)	(segid 3A4 and resid 359 and name CA)	12.50	0.22	0.22
	assign (segid 3A4 and resid 311 and name CA)	(segid 3A4 and resid 359 and name CB)	12.58	0.23	0.23
	assign (segid 3A4 and resid 311 and name CA)	(segid 3A4 and resid 360 and name CA)	10.28	0.16	0.15
	assign (segid 3A4 and resid 311 and name CA)	(segid 3A4 and resid 360 and name CB)	11.12	0.18	0.18
	assign (segid 3A4 and resid 311 and name CA)	(segid 3A4 and resid 361 and name CA)	10.96	0.19	0.18
25	assign (segid 3A4 and resid 311 and name CA)	(segid 3A4 and resid 361 and name CB)	12.41	0.21	0.20
	assign (segid 3A4 and resid 311 and name CA)	(segid 3A4 and resid 362 and name CA)	9.74	0.13	0.13
	assign (segid 3A4 and resid 311 and name CA)	(segid 3A4 and resid 362 and name CB)	10.44	0.13	0.14
	assign (segid 3A4 and resid 311 and name CA)	(segid 3A4 and resid 362 and name O)	7.46	0.13	0.14
	assign (segid 3A4 and resid 311 and name CA)	(segid 3A4 and resid 363 and name C)	7.00	0.07	0.07
30	assign (segid 3A4 and resid 311 and name CA)	(segid 3A4 and resid 363 and name CA)	6.89	0.10	0.09
	assign (segid 3A4 and resid 311 and name CA)	(segid 3A4 and resid 363 and name CB)	7.17	0.16	0.16
	assign (segid 3A4 and resid 311 and name CA)	(segid 3A4 and resid 363 and name CG)	6.27	0.19	0.19
	assign (segid 3A4 and resid 311 and name CA)	(segid 3A4 and resid 364 and name C)	5.88	0.08	0.08
	assign (segid 3A4 and resid 311 and name CA)	(segid 3A4 and resid 364 and name CA)	6.78	0.05	0.06
35	assign (segid 3A4 and resid 311 and name CA)	(segid 3A4 and resid 364 and name CB)	7.75	0.04	0.04
	assign (segid 3A4 and resid 311 and name CA)	(segid 3A4 and resid 364 and name N)	6.27	0.07	0.06
	assign (segid 3A4 and resid 311 and name CA)	(segid 3A4 and resid 364 and name O)	5.41	0.15	0.14
	assign (segid 3A4 and resid 311 and name CA)	(segid 3A4 and resid 365 and name C)	6.39	0.17	0.16
	assign (segid 3A4 and resid 311 and name CA)	(segid 3A4 and resid 365 and name CA)	5.63	0.19	0.19
40	assign (segid 3A4 and resid 311 and name CA)	(segid 3A4 and resid 365 and name CB)	6.34	0.19	0.20
	assign (segid 3A4 and resid 311 and name CA)	(segid 3A4 and resid 365 and name N)	6.01	0.15	0.15
	assign (segid 3A4 and resid 311 and name CA)	(segid 3A4 and resid 365 and name O)	6.31	0.19	0.19
	assign (segid 3A4 and resid 311 and name CA)	(segid 3A4 and resid 381 and name CA)	9.02	0.40	0.40
	assign (segid 3A4 and resid 311 and name CA)	(segid 3A4 and resid 382 and name CA)	11.54	0.25	0.24
45	assign (segid 3A4 and resid 311 and name CA)	(segid 3A4 and resid 382 and name CB)	12.76	0.31	0.31
	assign (segid 3A4 and resid 311 and name CA)	(segid 3A4 and resid 383 and name CA)	10.23	0.30	0.30
	assign (segid 3A4 and resid 311 and name CA)	(segid 3A4 and resid 384 and name CA)	12.85	0.44	0.45
	assign (segid 3A4 and resid 311 and name CA)	(segid 3A4 and resid 384 and name CB)	12.75	0.52	0.53
	assign (segid 3A4 and resid 311 and name CA)	(segid 3A4 and resid 385 and name CA)	15.35	0.41	0.40
50	assign (segid 3A4 and resid 311 and name CA)	(segid 3A4 and resid 386 and name CA)	17.29	0.50	0.51
	assign (segid 3A4 and resid 311 and name CA)	(segid 3A4 and resid 390 and name CA)	18.33	0.47	0.47
	assign (segid 3A4 and resid 311 and name CA)	(segid 3A4 and resid 390 and name CB)	17.99	0.43	0.42
	assign (segid 3A4 and resid 311 and name CA)	(segid 3A4 and resid 391 and name CA)	17.35	0.50	0.50
	assign (segid 3A4 and resid 311 and name CA)	(segid 3A4 and resid 391 and name CB)	16.02	0.50	0.50
55	assign (segid 3A4 and resid 311 and name CA)	(segid 3A4 and resid 393 and name CA)	18.05	0.52	0.52
	assign (segid 3A4 and resid 311 and name CA)	(segid 3A4 and resid 394 and name CA)	14.69	0.55	0.55
	assign (segid 3A4 and resid 311 and name CA)	(segid 3A4 and resid 394 and name CB)	14.45	0.65	0.64
	assign (segid 3A4 and resid 311 and name CA)	(segid 3A4 and resid 395 and name CA)	15.82	0.62	0.61
	assign (segid 3A4 and resid 311 and name CA)	(segid 3A4 and resid 396 and name CA)	17.11	0.51	0.52
60	assign (segid 3A4 and resid 311 and name CA)	(segid 3A4 and resid 396 and name CB)	18.29	0.53	0.54
	assign (segid 3A4 and resid 311 and name CA)	(segid 3A4 and resid 397 and name CA)	14.12	0.54	0.54
	assign (segid 3A4 and resid 311 and name CA)	(segid 3A4 and resid 397 and name CB)	13.59	0.58	0.57
	assign (segid 3A4 and resid 311 and name CA)	(segid 3A4 and resid 398 and name CA)	11.84	0.50	0.51
	assign (segid 3A4 and resid 311 and name CA)	(segid 3A4 and resid 398 and name CB)	11.59	0.56	0.56
65	assign (segid 3A4 and resid 311 and name CA)	(segid 3A4 and resid 399 and name CA)	14.82	0.42	0.43
	assign (segid 3A4 and resid 311 and name CA)	(segid 3A4 and resid 399 and name CB)	16.21	0.44	0.44
	assign (segid 3A4 and resid 311 and name CA)	(segid 3A4 and resid 400 and name CA)	15.43	0.40	0.40
	assign (segid 3A4 and resid 311 and name CA)	(segid 3A4 and resid 400 and name CB)	15.88	0.35	0.34
	assign (segid 3A4 and resid 311 and name CA)	(segid 3A4 and resid 401 and name CA)	12.03	0.42	0.41
70	assign (segid 3A4 and resid 311 and name CA)	(segid 3A4 and resid 402 and name CA)	12.19	0.36	0.36
	assign (segid 3A4 and resid 311 and name CA)	(segid 3A4 and resid 402 and name CB)	12.32	0.34	0.34
	assign (segid 3A4 and resid 311 and name CA)	(segid 3A4 and resid 403 and name CA)	15.87	0.37	0.36
	assign (segid 3A4 and resid 311 and name CA)	(segid 3A4 and resid 403 and name CB)	16.94	0.36	0.35
	assign (segid 3A4 and resid 311 and name CA)	(segid 3A4 and resid 404 and name CA)	15.70	0.51	0.52
75	assign (segid 3A4 and resid 311 and name CA)	(segid 3A4 and resid 404 and name CB)	15.32	0.63	0.64
	assign (segid 3A4 and resid 311 and name CA)	(segid 3A4 and resid 405 and name CA)	13.27	0.34	0.34
	assign (segid 3A4 and resid 311 and name CA)	(segid 3A4 and resid 405 and name CB)	11.78	0.35	0.34
	assign (segid 3A4 and resid 311 and name CA)	(segid 3A4 and resid 406 and name CA)	15.17	0.31	0.32
	assign (segid 3A4 and resid 311 and name CA)	(segid 3A4 and resid 407 and name CA)	18.39	0.28	0.29
80	assign (segid 3A4 and resid 311 and name CA)	(segid 3A4 and resid 407 and name CB)	19.08	0.34	0.34
	assign (segid 3A4 and resid 311 and name CA)	(segid 3A1 and resid 408 and name CA)	17.87	0.26	0.25
	assign (segid 3A4 and resid 311 and name CA)	(segid 3A4 and resid 408 and name CB)	16.93	0.31	0.32
	assign (segid 3A4 and resid 311 and name CA)	(segid 3A4 and resid 409 and name CA)	17.04	0.50	0.50

	assign (segid 3A4 and resid 311 and name CA)	(segid 3A4 and resid 409 and name CB)	15.80	0.54	0.55
	assign (segid 3A4 and resid 311 and name CA)	(segid 3A4 and resid 433 and name CA)	16.12	0.69	0.69
	assign (segid 3A4 and resid 311 and name CA)	(segid 3A4 and resid 434 and name CA)	15.99	1.00	1.00
	assign (segid 3A4 and resid 311 and name CA)	(segid 3A4 and resid 435 and name CA)	16.86	1.10	1.11
5	assign (segid 3A4 and resid 311 and name CB)	(segid 3A4 and resid 311 and name CD)	2.58	0.03	0.03
	assign (segid 3A4 and resid 311 and name CB)	(segid 3A4 and resid 311 and name CG)	1.53	0.01	0.01
	assign (segid 3A4 and resid 311 and name CB)	(segid 3A4 and resid 311 and name OE1)	2.83	0.04	0.04
	assign (segid 3A4 and resid 311 and name CB)	(segid 3A4 and resid 312 and name C)	5.52	0.04	0.03
	assign (segid 3A4 and resid 311 and name CB)	(segid 3A4 and resid 312 and name CA)	4.60	0.03	0.04
10	assign (segid 3A4 and resid 311 and name CB)	(segid 3A4 and resid 312 and name CB)	5.52	0.04	0.03
	assign (segid 3A4 and resid 311 and name CB)	(segid 3A4 and resid 312 and name N)	3.29	0.03	0.04
	assign (segid 3A4 and resid 311 and name CB)	(segid 3A4 and resid 312 and name O)	6.36	0.07	0.06
	assign (segid 3A4 and resid 311 and name CB)	(segid 3A4 and resid 313 and name C)	6.82	0.11	0.11
	assign (segid 3A4 and resid 311 and name CB)	(segid 3A4 and resid 313 and name CA)	6.86	0.06	0.06
15	assign (segid 3A4 and resid 311 and name CB)	(segid 3A4 and resid 313 and name CB)	7.39	0.09	0.10
	assign (segid 3A4 and resid 311 and name CB)	(segid 3A4 and resid 313 and name N)	5.70	0.04	0.04
	assign (segid 3A4 and resid 311 and name CB)	(segid 3A4 and resid 314 and name C)	6.68	0.08	0.09
	assign (segid 3A4 and resid 311 and name CB)	(segid 3A4 and resid 314 and name CA)	6.25	0.08	0.07
	assign (segid 3A4 and resid 311 and name CB)	(segid 3A4 and resid 314 and name CB)	5.47	0.09	0.08
20	assign (segid 3A4 and resid 311 and name CB)	(segid 3A4 and resid 314 and name CG)	6.43	0.07	0.07
	assign (segid 3A4 and resid 311 and name CB)	(segid 3A4 and resid 314 and name N)	5.82	0.10	0.10
	assign (segid 3A4 and resid 311 and name CB)	(segid 3A4 and resid 315 and name CA)	6.69	0.22	0.22
	assign (segid 3A4 and resid 311 and name CB)	(segid 3A4 and resid 315 and name CB)	6.00	0.30	0.29
	assign (segid 3A4 and resid 311 and name CB)	(segid 3A4 and resid 315 and name N)	5.93	0.13	0.14
25	assign (segid 3A4 and resid 311 and name CB)	(segid 3A4 and resid 316 and name CA)	9.32	0.18	0.18
	assign (segid 3A4 and resid 311 and name CB)	(segid 3A4 and resid 317 and name CA)	10.99	0.14	0.14
	assign (segid 3A4 and resid 311 and name CB)	(segid 3A4 and resid 318 and name CA)	13.74	0.34	0.34
	assign (segid 3A4 and resid 311 and name CB)	(segid 3A4 and resid 318 and name CB)	13.67	0.36	0.36
	assign (segid 3A4 and resid 311 and name CB)	(segid 3A4 and resid 319 and name CA)	16.31	0.34	0.35
30	assign (segid 3A4 and resid 311 and name CB)	(segid 3A4 and resid 319 and name CB)	16.56	0.28	0.28
	assign (segid 3A4 and resid 311 and name CB)	(segid 3A4 and resid 346 and name CA)	18.66	0.30	0.30
	assign (segid 3A4 and resid 311 and name CB)	(segid 3A4 and resid 346 and name CB)	18.99	0.23	0.23
	assign (segid 3A4 and resid 311 and name CB)	(segid 3A4 and resid 347 and name CA)	15.41	0.41	0.40
	assign (segid 3A4 and resid 311 and name CB)	(segid 3A4 and resid 347 and name CB)	15.16	0.48	0.48
35	assign (segid 3A4 and resid 311 and name CB)	(segid 3A4 and resid 348 and name CA)	13.71	0.38	0.38
	assign (segid 3A4 and resid 311 and name CB)	(segid 3A4 and resid 349 and name CA)	15.42	0.31	0.30
	assign (segid 3A4 and resid 311 and name CB)	(segid 3A4 and resid 349 and name CB)	16.91	0.31	0.30
	assign (segid 3A4 and resid 311 and name CB)	(segid 3A4 and resid 350 and name CA)	14.48	0.19	0.19
	assign (segid 3A4 and resid 311 and name CB)	(segid 3A4 and resid 350 and name CB)	14.77	0.31	0.30
40	assign (segid 3A4 and resid 311 and name CB)	(segid 3A4 and resid 351 and name CA)	10.75	0.16	0.15
	assign (segid 3A4 and resid 311 and name CB)	(segid 3A4 and resid 352 and name CA)	11.84	0.24	0.23
	assign (segid 3A4 and resid 311 and name CB)	(segid 3A4 and resid 352 and name CB)	12.37	0.21	0.21
	assign (segid 3A4 and resid 311 and name CB)	(segid 3A4 and resid 353 and name CA)	14.45	0.36	0.36
	assign (segid 3A4 and resid 311 and name CB)	(segid 3A4 and resid 353 and name CB)	14.99	0.41	0.41
45	assign (segid 3A4 and resid 311 and name CB)	(segid 3A4 and resid 354 and name CA)	15.03	0.45	0.46
	assign (segid 3A4 and resid 311 and name CB)	(segid 3A4 and resid 354 and name CB)	16.09	0.50	0.51
	assign (segid 3A4 and resid 311 and name CB)	(segid 3A4 and resid 355 and name CA)	16.78	0.55	0.56
	assign (segid 3A4 and resid 311 and name CB)	(segid 3A4 and resid 355 and name CB)	17.93	0.50	0.50
	assign (segid 3A4 and resid 311 and name CB)	(segid 3A4 and resid 356 and name CA)	13.88	0.50	0.49
50	assign (segid 3A4 and resid 311 and name CB)	(segid 3A4 and resid 356 and name CB)	13.60	0.46	0.46
	assign (segid 3A4 and resid 311 and name CB)	(segid 3A4 and resid 357 and name CA)	10.95	0.47	0.47
	assign (segid 3A4 and resid 311 and name CB)	(segid 3A4 and resid 357 and name CB)	9.83	0.51	0.50
	assign (segid 3A4 and resid 311 and name CB)	(segid 3A4 and resid 358 and name CA)	12.78	0.71	0.71
	assign (segid 3A4 and resid 311 and name CB)	(segid 3A4 and resid 358 and name CB)	13.31	1.05	1.06
55	assign (segid 3A4 and resid 311 and name CB)	(segid 3A4 and resid 359 and name CA)	11.99	0.23	0.23
	assign (segid 3A4 and resid 311 and name CB)	(segid 3A4 and resid 359 and name CB)	11.90	0.25	0.24
	assign (segid 3A4 and resid 311 and name CB)	(segid 3A4 and resid 360 and name CA)	10.19	0.15	0.14
	assign (segid 3A4 and resid 311 and name CB)	(segid 3A4 and resid 360 and name CB)	11.20	0.16	0.16
	assign (segid 3A4 and resid 311 and name CB)	(segid 3A4 and resid 361 and name CA)	10.76	0.17	0.16
60	assign (segid 3A4 and resid 311 and name CB)	(segid 3A4 and resid 361 and name CB)	12.21	0.18	0.19
	assign (segid 3A4 and resid 311 and name CB)	(segid 3A4 and resid 362 and name C)	7.52	0.13	0.14
	assign (segid 3A4 and resid 311 and name CB)	(segid 3A4 and resid 362 and name CA)	9.03	0.14	0.13
	assign (segid 3A4 and resid 311 and name CB)	(segid 3A4 and resid 362 and name CB)	9.59	0.13	0.13
	assign (segid 3A4 and resid 311 and name CB)	(segid 3A4 and resid 362 and name O)	6.77	0.13	0.14
65	assign (segid 3A4 and resid 311 and name CB)	(segid 3A4 and resid 363 and name C)	5.84	0.10	0.10
	assign (segid 3A4 and resid 311 and name CB)	(segid 3A4 and resid 363 and name CA)	5.98	0.13	0.13
	assign (segid 3A4 and resid 311 and name CB)	(segid 3A4 and resid 363 and name CB)	6.32	0.18	0.19
	assign (segid 3A4 and resid 311 and name CB)	(segid 3A4 and resid 363 and name CG)	5.40	0.23	0.23
	assign (segid 3A4 and resid 311 and name CB)	(segid 3A4 and resid 363 and name N)	7.26	0.14	0.13
70	assign (segid 3A4 and resid 311 and name CB)	(segid 3A4 and resid 363 and name O)	6.77	0.13	0.13
	assign (segid 3A4 and resid 311 and name CB)	(segid 3A4 and resid 364 and name C)	4.41	0.08	0.07
	assign (segid 3A4 and resid 311 and name CB)	(segid 3A4 and resid 364 and name CA)	5.38	0.05	0.06
	assign (segid 3A4 and resid 311 and name CB)	(segid 3A4 and resid 364 and name CB)	6.44	0.06	0.05
	assign (segid 3A4 and resid 311 and name CB)	(segid 3A4 and resid 364 and name N)	5.02	0.07	0.07
75	assign (segid 3A4 and resid 311 and name CB)	(segid 3A4 and resid 364 and name O)	4.05	0.16	0.17
	assign (segid 3A4 and resid 311 and name CB)	(segid 3A4 and resid 365 and name C)	5.03	0.12	0.13
	assign (segid 3A4 and resid 311 and name CB)	(segid 3A4 and resid 365 and name CA)	4.17	0.16	0.15
	assign (segid 3A4 and resid 311 and name CB)	(segid 3A4 and resid 365 and name CB)	4.95	0.19	0.18
	assign (segid 3A4 and resid 311 and name CB)	(segid 3A4 and resid 365 and name N)	1.48	0.14	0.13
80	assign (segid 3A4 and resid 311 and name CB)	(segid 3A4 and resid 365 and name O)	5.14	0.15	0.15
	assign (segid 3A4 and resid 311 and name CB)	(segid 3A4 and resid 381 and name CA)	10.22	0.40	0.41
	assign (segid 3A4 and resid 311 and name CB)	(segid 3A4 and resid 382 and name CA)	12.93	0.26	0.26
	assign (segid 3A4 and resid 311 and name CB)	(segid 3A4 and resid 382 and name CB)	14.12	0.33	0.33

	assign (segid 3A4 and resid 311 and name CB) (segid 3A4 and resid 383 and name CA)	11.74	0.31	0.32
	assign (segid 3A4 and resid 311 and name CB) (segid 3A4 and resid 384 and name CA)	14.38	0.45	0.45
	assign (segid 3A4 and resid 311 and name CB) (segid 3A4 and resid 384 and name CB)	14.25	0.53	0.53
	assign (segid 3A4 and resid 311 and name CB) (segid 3A4 and resid 385 and name CA)	16.84	0.41	0.42
5	assign (segid 3A4 and resid 311 and name CB) (segid 3A4 and resid 386 and name CA)	18.70	0.52	0.53
	assign (segid 3A4 and resid 311 and name CB) (segid 3A4 and resid 391 and name CA)	18.84	0.51	0.51
	assign (segid 3A4 and resid 311 and name CB) (segid 3A4 and resid 391 and name CB)	17.51	0.51	0.51
	assign (segid 3A4 and resid 311 and name CB) (segid 3A4 and resid 394 and name CA)	16.02	0.57	0.57
	assign (segid 3A4 and resid 311 and name CB) (segid 3A4 and resid 394 and name CB)	15.80	0.67	0.66
10	assign (segid 3A4 and resid 311 and name CB) (segid 3A4 and resid 395 and name CA)	16.95	0.65	0.64
	assign (segid 3A4 and resid 311 and name CB) (segid 3A4 and resid 396 and name CA)	18.21	0.53	0.53
	assign (segid 3A4 and resid 311 and name CB) (segid 3A4 and resid 397 and name CA)	15.28	0.56	0.56
	assign (segid 3A4 and resid 311 and name CB) (segid 3A4 and resid 397 and name CB)	14.84	0.60	0.59
	assign (segid 3A4 and resid 311 and name CB) (segid 3A4 and resid 398 and name CA)	12.83	0.53	0.53
15	assign (segid 3A4 and resid 311 and name CB) (segid 3A4 and resid 398 and name CB)	12.58	0.59	0.60
	assign (segid 3A4 and resid 311 and name CB) (segid 3A4 and resid 399 and name CA)	15.58	0.44	0.44
	assign (segid 3A4 and resid 311 and name CB) (segid 3A4 and resid 399 and name CB)	17.00	0.45	0.45
	assign (segid 3A4 and resid 311 and name CB) (segid 3A4 and resid 400 and name CA)	16.19	0.40	0.40
	assign (segid 3A4 and resid 311 and name CB) (segid 3A4 and resid 400 and name CB)	16.73	0.34	0.34
20	assign (segid 3A4 and resid 311 and name CB) (segid 3A4 and resid 401 and name CA)	12.69	0.42	0.42
	assign (segid 3A4 and resid 311 and name CB) (segid 3A4 and resid 402 and name CA)	12.54	0.38	0.37
	assign (segid 3A4 and resid 311 and name CB) (segid 3A4 and resid 402 and name CB)	12.69	0.34	0.34
	assign (segid 3A4 and resid 311 and name CB) (segid 3A4 and resid 403 and name CA)	16.16	0.38	0.37
	assign (segid 3A4 and resid 311 and name CB) (segid 3A4 and resid 403 and name CB)	17.33	0.37	0.37
25	assign (segid 3A4 and resid 311 and name CB) (segid 3A4 and resid 404 and name CA)	15.97	0.54	0.55
	assign (segid 3A4 and resid 311 and name CB) (segid 3A4 and resid 404 and name CB)	15.69	0.66	0.67
	assign (segid 3A4 and resid 311 and name CB) (segid 3A4 and resid 405 and name CA)	13.26	0.40	0.39
	assign (segid 3A4 and resid 311 and name CB) (segid 3A4 and resid 405 and name CB)	11.76	0.40	0.40
	assign (segid 3A4 and resid 311 and name CB) (segid 3A4 and resid 406 and name CA)	14.97	0.28	0.28
30	assign (segid 3A4 and resid 311 and name CB) (segid 3A4 and resid 407 and name CA)	18.26	0.30	0.30
	assign (segid 3A4 and resid 311 and name CB) (segid 3A4 and resid 407 and name CB)	19.05	0.36	0.36
	assign (segid 3A4 and resid 311 and name CB) (segid 3A4 and resid 408 and name CA)	17.67	0.33	0.33
	assign (segid 3A4 and resid 311 and name CB) (segid 3A4 and resid 408 and name CB)	16.79	0.39	0.39
	assign (segid 3A4 and resid 311 and name CB) (segid 3A4 and resid 409 and name CA)	16.53	0.52	0.53
35	assign (segid 3A4 and resid 311 and name CB) (segid 3A4 and resid 409 and name CB)	15.24	0.56	0.55
	assign (segid 3A4 and resid 311 and name CB) (segid 3A4 and resid 410 and name CA)	19.28	0.37	0.37
	assign (segid 3A4 and resid 311 and name CB) (segid 3A4 and resid 433 and name CA)	17.15	0.76	0.76
	assign (segid 3A4 and resid 311 and name CB) (segid 3A4 and resid 434 and name CA)	16.85	1.02	1.02
	assign (segid 3A4 and resid 311 and name CB) (segid 3A4 and resid 435 and name CA)	17.45	1.15	1.15
40	assign (segid 3A4 and resid 311 and name CD) (segid 3A4 and resid 311 and name OE1)	1.24	0.01	0.01
	assign (segid 3A4 and resid 311 and name CD) (segid 3A4 and resid 312 and name C)	6.50	0.10	0.11
	assign (segid 3A4 and resid 311 and name CD) (segid 3A4 and resid 312 and name CA)	5.87	0.10	0.11
	assign (segid 3A4 and resid 311 and name CD) (segid 3A4 and resid 312 and name CB)	7.11	0.10	0.10
	assign (segid 3A4 and resid 311 and name CD) (segid 3A4 and resid 312 and name N)	4.90	0.09	0.10
45	assign (segid 3A4 and resid 311 and name CD) (segid 3A4 and resid 312 and name O)	6.96	0.16	0.15
	assign (segid 3A4 and resid 311 and name CD) (segid 3A4 and resid 313 and name C)	7.27	0.13	0.13
	assign (segid 3A4 and resid 311 and name CD) (segid 3A4 and resid 313 and name CA)	7.80	0.10	0.10
	assign (segid 3A4 and resid 311 and name CD) (segid 3A4 and resid 313 and name N)	6.89	0.09	0.08
	assign (segid 3A4 and resid 311 and name CD) (segid 3A4 and resid 314 and name C)	5.99	0.17	0.17
50	assign (segid 3A4 and resid 311 and name CD) (segid 3A4 and resid 314 and name CA)	5.92	0.11	0.11
	assign (segid 3A4 and resid 311 and name CD) (segid 3A4 and resid 314 and name CB)	4.88	0.10	0.11
	assign (segid 3A4 and resid 311 and name CD) (segid 3A4 and resid 314 and name CG)	5.29	0.07	0.07
	assign (segid 3A4 and resid 311 and name CD) (segid 3A4 and resid 314 and name N)	6.09	0.11	0.11
	assign (segid 3A4 and resid 311 and name CD) (segid 3A4 and resid 314 and name O)	6.99	0.22	0.23
55	assign (segid 3A4 and resid 311 and name CD) (segid 3A4 and resid 315 and name C)	7.14	0.27	0.26
	assign (segid 3A4 and resid 311 and name CD) (segid 3A4 and resid 315 and name CA)	5.70	0.31	0.31
	assign (segid 3A4 and resid 311 and name CD) (segid 3A4 and resid 315 and name CB)	5.02	0.33	0.34
	assign (segid 3A4 and resid 311 and name CD) (segid 3A4 and resid 315 and name N)	5.23	0.20	0.20
	assign (segid 3A4 and resid 311 and name CD) (segid 3A4 and resid 351 and name O)	7.75	0.09	0.09
60	assign (segid 3A4 and resid 311 and name CD) (segid 3A4 and resid 359 and name O)	7.27	0.23	0.24
	assign (segid 3A4 and resid 311 and name CD) (segid 3A4 and resid 360 and name C)	7.34	0.10	0.09
	assign (segid 3A4 and resid 311 and name CD) (segid 3A4 and resid 360 and name CA)	7.66	0.12	0.13
	assign (segid 3A4 and resid 311 and name CD) (segid 3A4 and resid 360 and name O)	6.51	0.11	0.11
	assign (segid 3A4 and resid 311 and name CD) (segid 3A4 and resid 362 and name C)	5.39	0.08	0.09
65	assign (segid 3A4 and resid 311 and name CD) (segid 3A4 and resid 362 and name CA)	6.82	0.09	0.09
	assign (segid 3A4 and resid 311 and name CD) (segid 3A4 and resid 362 and name CB)	7.37	0.12	0.12
	assign (segid 3A4 and resid 311 and name CD) (segid 3A4 and resid 362 and name N)	7.12	0.13	0.13
	assign (segid 3A4 and resid 311 and name CD) (segid 3A4 and resid 362 and name O)	4.45	0.10	0.10
70	assign (segid 3A4 and resid 311 and name CD) (segid 3A4 and resid 363 and name C)	4.53	0.06	0.06
	assign (segid 3A4 and resid 311 and name CD) (segid 3A4 and resid 363 and name CA)	4.50	0.04	0.04
	assign (segid 3A4 and resid 311 and name CD) (segid 3A4 and resid 363 and name CB)	5.35	0.10	0.11
	assign (segid 3A4 and resid 311 and name CD) (segid 3A4 and resid 363 and name CG)	5.04	0.14	0.15
	assign (segid 3A4 and resid 311 and name CD) (segid 3A4 and resid 363 and name N)	5.47	0.06	0.06
	assign (segid 3A4 and resid 311 and name CD) (segid 3A4 and resid 363 and name O)	5.68	0.07	0.08
75	assign (segid 3A4 and resid 311 and name CD) (segid 3A4 and resid 364 and name C)	3.94	0.11	0.10
	assign (segid 3A4 and resid 311 and name CD) (segid 3A4 and resid 364 and name CA)	4.37	0.06	0.05
	assign (segid 3A4 and resid 311 and name CD) (segid 3A4 and resid 364 and name CB)	5.04	0.03	0.03
	assign (segid 3A4 and resid 311 and name CD) (segid 3A4 and resid 364 and name N)	3.64	0.04	0.05
	assign (segid 3A4 and resid 311 and name CD) (segid 3A4 and resid 364 and name O)	3.43	0.15	0.15
80	assign (segid 3A4 and resid 311 and name CD) (segid 3A4 and resid 365 and name C)	5.75	0.25	0.25
	assign (segid 3A4 and resid 311 and name CD) (segid 3A4 and resid 365 and name CA)	5.05	0.21	0.22
	assign (segid 3A4 and resid 311 and name CD) (segid 3A4 and resid 365 and name CB)	6.24	0.20	0.20
	assign (segid 3A4 and resid 311 and name CD) (segid 3A4 and resid 365 and name N)	4.71	0.17	0.16

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	assign (segid 3A4 and resid 311 and name O) (segid 3A4 and resid 312 and name CA)	2.74	0.06	0.05
	assign (segid 3A4 and resid 311 and name O) (segid 3A4 and resid 312 and name CB)	4.22	0.07	0.06
	assign (segid 3A4 and resid 311 and name O) (segid 3A4 and resid 312 and name N)	2.23	0.01	0.02
	assign (segid 3A4 and resid 311 and name O) (segid 3A4 and resid 312 and name O)	3.44	0.07	0.07
5	assign (segid 3A4 and resid 311 and name O) (segid 3A4 and resid 313 and name C)	4.14	0.11	0.12
	assign (segid 3A4 and resid 311 and name O) (segid 3A4 and resid 313 and name CA)	4.46	0.07	0.07
	assign (segid 3A4 and resid 311 and name O) (segid 3A4 and resid 313 and name CB)	5.50	0.07	0.06
	assign (segid 3A4 and resid 311 and name O) (segid 3A4 and resid 313 and name CG)	6.48	0.16	0.17
	assign (segid 3A4 and resid 311 and name O) (segid 3A4 and resid 313 and name N)	3.50	0.05	0.05
10	assign (segid 3A4 and resid 311 and name O) (segid 3A4 and resid 313 and name O)	5.11	0.15	0.15
	assign (segid 3A4 and resid 311 and name O) (segid 3A4 and resid 314 and name C)	3.80	0.09	0.09
	assign (segid 3A4 and resid 311 and name O) (segid 3A4 and resid 314 and name CA)	3.74	0.08	0.09
	assign (segid 3A4 and resid 311 and name O) (segid 3A4 and resid 314 and name CB)	3.64	0.10	0.10
	assign (segid 3A4 and resid 311 and name O) (segid 3A4 and resid 314 and name CG)	4.82	0.13	0.12
15	assign (segid 3A4 and resid 311 and name O) (segid 3A4 and resid 314 and name N)	3.28	0.09	0.10
	assign (segid 3A4 and resid 311 and name O) (segid 3A4 and resid 314 and name O)	4.98	0.10	0.10
	assign (segid 3A4 and resid 311 and name O) (segid 3A4 and resid 315 and name C)	4.77	0.15	0.15
	assign (segid 3A4 and resid 311 and name O) (segid 3A4 and resid 315 and name CA)	3.71	0.16	0.17
	assign (segid 3A4 and resid 311 and name O) (segid 3A4 and resid 315 and name CB)	3.35	0.20	0.19
20	assign (segid 3A4 and resid 311 and name O) (segid 3A4 and resid 315 and name N)	2.89	0.13	0.12
	assign (segid 3A4 and resid 311 and name O) (segid 3A4 and resid 315 and name O)	5.93	0.16	0.15
	assign (segid 3A4 and resid 311 and name O) (segid 3A4 and resid 316 and name C)	6.74	0.16	0.15
	assign (segid 3A4 and resid 311 and name O) (segid 3A4 and resid 316 and name CA)	6.12	0.18	0.18
	assign (segid 3A4 and resid 311 and name O) (segid 3A4 and resid 316 and name N)	4.76	0.17	0.18
25	assign (segid 3A4 and resid 311 and name O) (segid 3A4 and resid 317 and name N)	6.90	0.26	0.26
	assign (segid 3A4 and resid 311 and name O) (segid 3A4 and resid 360 and name O)	7.59	0.23	0.22
	assign (segid 3A4 and resid 311 and name O) (segid 3A4 and resid 362 and name C)	7.44	0.13	0.14
	assign (segid 3A4 and resid 311 and name O) (segid 3A4 and resid 362 and name O)	6.77	0.12	0.12
	assign (segid 3A4 and resid 311 and name O) (segid 3A4 and resid 363 and name C)	6.80	0.10	0.11
30	assign (segid 3A4 and resid 311 and name O) (segid 3A4 and resid 363 and name CA)	6.18	0.10	0.10
	assign (segid 3A4 and resid 311 and name O) (segid 3A4 and resid 363 and name CB)	6.27	0.17	0.17
	assign (segid 3A4 and resid 311 and name O) (segid 3A4 and resid 363 and name CG)	5.57	0.13	0.12
	assign (segid 3A4 and resid 311 and name O) (segid 3A4 and resid 363 and name N)	7.24	0.12	0.12
	assign (segid 3A4 and resid 311 and name O) (segid 3A4 and resid 364 and name C)	6.92	0.16	0.16
35	assign (segid 3A4 and resid 311 and name O) (segid 3A4 and resid 364 and name CA)	7.38	0.14	0.15
	assign (segid 3A4 and resid 311 and name O) (segid 3A4 and resid 364 and name N)	6.43	0.14	0.14
	assign (segid 3A4 and resid 311 and name O) (segid 3A4 and resid 364 and name O)	6.64	0.23	0.23
	assign (segid 3A4 and resid 311 and name O) (segid 3A4 and resid 365 and name CA)	7.25	0.17	0.16
	assign (segid 3A4 and resid 311 and name O) (segid 3A4 and resid 365 and name N)	7.23	0.15	0.14
40	assign (segid 3A4 and resid 311 and name OE1) (segid 3A4 and resid 312 and name C)	6.60	0.07	0.08
	assign (segid 3A4 and resid 311 and name OE1) (segid 3A4 and resid 312 and name CA)	6.18	0.09	0.10
	assign (segid 3A4 and resid 311 and name OE1) (segid 3A4 and resid 312 and name CB)	7.48	0.09	0.08
	assign (segid 3A4 and resid 311 and name OE1) (segid 3A4 and resid 312 and name N)	5.11	0.09	0.10
	assign (segid 3A4 and resid 311 and name OE1) (segid 3A4 and resid 312 and name O)	7.11	0.12	0.11
45	assign (segid 3A4 and resid 311 and name OE1) (segid 3A4 and resid 313 and name C)	6.90	0.07	0.07
	assign (segid 3A4 and resid 311 and name OE1) (segid 3A4 and resid 313 and name CA)	7.52	0.05	0.06
	assign (segid 3A4 and resid 311 and name OE1) (segid 3A4 and resid 313 and name N)	6.76	0.05	0.06
	assign (segid 3A4 and resid 311 and name OE1) (segid 3A4 and resid 313 and name O)	7.76	0.12	0.11
	assign (segid 3A4 and resid 311 and name OE1) (segid 3A4 and resid 314 and name C)	5.67	0.14	0.14
50	assign (segid 3A4 and resid 311 and name OE1) (segid 3A4 and resid 314 and name CA)	5.36	0.07	0.06
	assign (segid 3A4 and resid 311 and name OE1) (segid 3A4 and resid 314 and name CB)	4.12	0.07	0.08
	assign (segid 3A4 and resid 311 and name OE1) (segid 3A4 and resid 314 and name CG)	4.47	0.06	0.06
	assign (segid 3A4 and resid 311 and name OE1) (segid 3A4 and resid 314 and name N)	5.63	0.07	0.07
	assign (segid 3A4 and resid 311 and name OE1) (segid 3A4 and resid 314 and name O)	6.67	0.20	0.20
55	assign (segid 3A4 and resid 311 and name OE1) (segid 3A4 and resid 315 and name C)	7.34	0.25	0.24
	assign (segid 3A4 and resid 311 and name OE1) (segid 3A4 and resid 315 and name CA)	5.88	0.28	0.29
	assign (segid 3A4 and resid 311 and name OE1) (segid 3A4 and resid 315 and name CB)	5.51	0.31	0.31
	assign (segid 3A4 and resid 311 and name OE1) (segid 3A4 and resid 315 and name N)	5.17	0.19	0.19
	assign (segid 3A4 and resid 311 and name OE1) (segid 3A4 and resid 351 and name O)	7.15	0.12	0.11
60	assign (segid 3A4 and resid 311 and name OE1) (segid 3A4 and resid 357 and name CB)	7.02	0.48	0.48
	assign (segid 3A4 and resid 311 and name OE1) (segid 3A4 and resid 360 and name C)	7.52	0.09	0.08
	assign (segid 3A4 and resid 311 and name OE1) (segid 3A4 and resid 360 and name CA)	7.64	0.12	0.12
	assign (segid 3A4 and resid 311 and name OE1) (segid 3A4 and resid 360 and name O)	6.70	0.11	0.12
	assign (segid 3A4 and resid 311 and name OE1) (segid 3A4 and resid 362 and name C)	6.29	0.05	0.06
65	assign (segid 3A4 and resid 311 and name OE1) (segid 3A4 and resid 362 and name CA)	7.64	0.07	0.06
	assign (segid 3A4 and resid 311 and name OE1) (segid 3A4 and resid 362 and name N)	7.77	0.10	0.11
	assign (segid 3A4 and resid 311 and name OE1) (segid 3A4 and resid 362 and name O)	5.23	0.07	0.08
	assign (segid 3A4 and resid 311 and name OE1) (segid 3A4 and resid 363 and name C)	5.69	0.08	0.08
	assign (segid 3A4 and resid 311 and name OE1) (segid 3A4 and resid 363 and name CA)	5.67	0.04	0.04
70	assign (segid 3A4 and resid 311 and name OE1) (segid 3A4 and resid 363 and name CB)	6.56	0.12	0.11
	assign (segid 3A4 and resid 311 and name OE1) (segid 3A4 and resid 363 and name CG)	6.24	0.15	0.15
	assign (segid 3A4 and resid 311 and name OE1) (segid 3A4 and resid 363 and name N)	6.53	0.05	0.05
	assign (segid 3A4 and resid 311 and name OE1) (segid 3A4 and resid 363 and name O)	6.84	0.10	0.09
	assign (segid 3A4 and resid 311 and name OE1) (segid 3A4 and resid 364 and name C)	4.68	0.13	0.14
75	assign (segid 3A4 and resid 311 and name OE1) (segid 3A4 and resid 364 and name CA)	5.28	0.08	0.08
	assign (segid 3A4 and resid 311 and name OE1) (segid 3A4 and resid 364 and name CB)	5.76	0.10	0.09
	assign (segid 3A4 and resid 311 and name OE1) (segid 3A4 and resid 364 and name N)	4.72	0.06	0.07
	assign (segid 3A4 and resid 311 and name OE1) (segid 3A4 and resid 364 and name O)	3.90	0.14	0.14
	assign (segid 3A4 and resid 311 and name OE1) (segid 3A4 and resid 365 and name C)	6.02	0.35	0.35
80	assign (segid 3A4 and resid 311 and name OE1) (segid 3A4 and resid 365 and name CA)	5.57	0.31	0.31
	assign (segid 3A4 and resid 311 and name OE1) (segid 3A4 and resid 365 and name CB)	6.83	0.30	0.29
	assign (segid 3A4 and resid 311 and name OE1) (segid 3A4 and resid 365 and name N)	5.46	0.23	0.23
	assign (segid 3A4 and resid 311 and name OE1) (segid 3A4 and resid 365 and name O)	6.22	0.44	0.43

	assign	(segid 3A4 and resid 312 and name C)	(segid 3A4 and resid 312 and name CB)	2.50	0.03	0.03
	assign	(segid 3A4 and resid 312 and name C)	(segid 3A4 and resid 312 and name O)	1.23	0.01	0.01
	assign	(segid 3A4 and resid 312 and name C)	(segid 3A4 and resid 313 and name C)	3.05	0.04	0.04
	assign	(segid 3A4 and resid 312 and name C)	(segid 3A4 and resid 313 and name CA)	2.44	0.02	0.01
5	assign	(segid 3A4 and resid 312 and name C)	(segid 3A4 and resid 313 and name CB)	3.71	0.02	0.01
	assign	(segid 3A4 and resid 312 and name C)	(segid 3A4 and resid 313 and name CG)	4.28	0.12	0.13
	assign	(segid 3A4 and resid 312 and name C)	(segid 3A4 and resid 313 and name N)	1.33	0.01	0.00
	assign	(segid 3A4 and resid 312 and name C)	(segid 3A4 and resid 313 and name O)	3.98	0.10	0.10
	assign	(segid 3A4 and resid 312 and name C)	(segid 3A4 and resid 314 and name C)	4.56	0.07	0.07
10	assign	(segid 3A4 and resid 312 and name C)	(segid 3A4 and resid 314 and name CA)	4.46	0.07	0.07
	assign	(segid 3A4 and resid 312 and name C)	(segid 3A4 and resid 314 and name CB)	5.23	0.08	0.08
	assign	(segid 3A4 and resid 312 and name C)	(segid 3A4 and resid 314 and name CG)	6.61	0.09	0.10
	assign	(segid 3A4 and resid 312 and name C)	(segid 3A4 and resid 314 and name N)	3.26	0.06	0.07
	assign	(segid 3A4 and resid 312 and name C)	(segid 3A4 and resid 314 and name O)	5.52	0.07	0.08
	assign	(segid 3A4 and resid 312 and name C)	(segid 3A4 and resid 315 and name C)	4.87	0.06	0.06
15	assign	(segid 3A4 and resid 312 and name C)	(segid 3A4 and resid 315 and name CA)	4.69	0.07	0.06
	assign	(segid 3A4 and resid 312 and name C)	(segid 3A4 and resid 315 and name CB)	4.67	0.10	0.11
	assign	(segid 3A4 and resid 312 and name C)	(segid 3A4 and resid 315 and name N)	3.95	0.07	0.08
	assign	(segid 3A4 and resid 312 and name C)	(segid 3A4 and resid 315 and name O)	6.08	0.07	0.06
	assign	(segid 3A4 and resid 312 and name C)	(segid 3A4 and resid 316 and name C)	5.22	0.32	0.33
20	assign	(segid 3A4 and resid 312 and name C)	(segid 3A4 and resid 316 and name CA)	4.89	0.16	0.16
	assign	(segid 3A4 and resid 312 and name C)	(segid 3A4 and resid 316 and name N)	4.05	0.11	0.11
	assign	(segid 3A4 and resid 312 and name C)	(segid 3A4 and resid 316 and name O)	5.53	0.87	0.87
	assign	(segid 3A4 and resid 312 and name C)	(segid 3A4 and resid 317 and name C)	7.41	0.27	0.26
	assign	(segid 3A4 and resid 312 and name C)	(segid 3A4 and resid 317 and name CA)	6.45	0.31	0.31
25	assign	(segid 3A4 and resid 312 and name C)	(segid 3A4 and resid 317 and name N)	5.61	0.19	0.19
	assign	(segid 3A4 and resid 312 and name C)	(segid 3A4 and resid 363 and name CG)	7.24	0.17	0.16
	assign	(segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 312 and name C)	1.54	0.02	0.01
	assign	(segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 312 and name CB)	1.53	0.01	0.00
30	assign	(segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 312 and name O)	2.39	0.03	0.04
	assign	(segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 313 and name C)	4.43	0.03	0.04
	assign	(segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 313 and name CA)	3.83	0.02	0.03
	assign	(segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 313 and name CB)	4.88	0.03	0.03
	assign	(segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 313 and name CG)	5.26	0.16	0.16
	assign	(segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 313 and name N)	2.46	0.03	0.02
35	assign	(segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 313 and name O)	5.44	0.09	0.09
	assign	(segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 314 and name C)	5.48	0.09	0.09
	assign	(segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 314 and name CA)	5.42	0.08	0.08
	assign	(segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 314 and name CB)	5.84	0.09	0.10
	assign	(segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 314 and name CG)	7.21	0.12	0.12
40	assign	(segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 314 and name N)	4.33	0.06	0.06
	assign	(segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 314 and name O)	6.54	0.08	0.08
	assign	(segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 315 and name C)	5.59	0.11	0.11
	assign	(segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 315 and name CA)	5.18	0.08	0.09
45	assign	(segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 315 and name CB)	4.71	0.10	0.10
	assign	(segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 315 and name N)	4.61	0.09	0.10
	assign	(segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 315 and name O)	6.79	0.12	0.12
	assign	(segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 316 and name C)	6.45	0.29	0.29
	assign	(segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 316 and name CA)	5.87	0.20	0.20
50	assign	(segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 316 and name N)	4.94	0.14	0.14
	assign	(segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 317 and name CA)	7.88	0.27	0.26
	assign	(segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 317 and name N)	6.94	0.18	0.19
	assign	(segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 318 and name CA)	9.85	0.41	0.40
	assign	(segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 318 and name CB)	9.57	0.38	0.38
55	assign	(segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 319 and name CA)	12.89	0.40	0.39
	assign	(segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 319 and name CB)	13.24	0.32	0.32
	assign	(segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 346 and name CA)	16.90	0.45	0.46
	assign	(segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 346 and name CB)	17.31	0.47	0.48
	assign	(segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 347 and name CA)	13.79	0.46	0.45
60	assign	(segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 347 and name CB)	13.28	0.50	0.49
	assign	(segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 348 and name CA)	11.90	0.56	0.57
	assign	(segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 349 and name CA)	14.52	0.61	0.61
	assign	(segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 349 and name CB)	15.97	0.60	0.59
	assign	(segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 350 and name CA)	14.31	0.29	0.29
65	assign	(segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 350 and name CB)	14.49	0.34	0.35
	assign	(segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 351 and name CA)	10.80	0.20	0.20
	assign	(segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 352 and name CA)	12.19	0.38	0.38
	assign	(segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 352 and name CB)	12.30	0.36	0.36
	assign	(segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 353 and name CA)	15.46	0.39	0.38
70	assign	(segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 353 and name CB)	15.99	0.38	0.38
	assign	(segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 354 and name CA)	16.88	0.51	0.50
	assign	(segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 354 and name CB)	17.88	0.56	0.57
	assign	(segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 355 and name CA)	18.98	0.48	0.47
	assign	(segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 356 and name CA)	16.23	0.48	0.48
75	assign	(segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 356 and name CB)	15.62	0.48	0.48
	assign	(segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 357 and name CA)	13.63	0.46	0.47
	assign	(segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 357 and name CB)	12.25	0.51	0.50
	assign	(segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 358 and name CA)	15.72	0.55	0.54
	assign	(segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 358 and name CB)	16.52	0.80	0.80
80	assign	(segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 359 and name CA)	14.47	0.29	0.29
	assign	(segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 359 and name CB)	14.61	0.29	0.29
	assign	(segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 360 and name CA)	11.85	0.25	0.26
	assign	(segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 360 and name CB)	12.61	0.29	0.28

	assign (segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 361 and name CA)	11.46	0.34	0.35
	assign (segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 361 and name CB)	12.72	0.38	0.38
	assign (segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 362 and name CA)	10.68	0.24	0.25
	assign (segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 362 and name CB)	11.76	0.18	0.18
5	assign (segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 363 and name CA)	7.58	0.14	0.14
	assign (segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 363 and name CB)	7.13	0.23	0.23
	assign (segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 363 and name CG)	6.06	0.17	0.17
	assign (segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 364 and name CA)	8.92	0.13	0.13
	assign (segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 364 and name CB)	10.15	0.12	0.13
10	assign (segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 365 and name CA)	8.14	0.14	0.15
	assign (segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 365 and name CB)	8.32	0.16	0.16
	assign (segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 381 and name CA)	10.79	0.41	0.40
	assign (segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 382 and name CA)	12.28	0.27	0.27
	assign (segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 382 and name CB)	13.49	0.32	0.33
15	assign (segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 383 and name CA)	9.87	0.31	0.32
	assign (segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 384 and name CA)	12.47	0.40	0.40
	assign (segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 384 and name CB)	12.54	0.46	0.46
	assign (segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 385 and name CA)	15.31	0.34	0.34
	assign (segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 386 and name CA)	17.93	0.41	0.42
20	assign (segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 390 and name CA)	18.31	0.39	0.39
	assign (segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 390 and name CB)	18.25	0.37	0.38
	assign (segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 391 and name CA)	16.72	0.43	0.42
	assign (segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 391 and name CB)	15.26	0.42	0.42
	assign (segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 392 and name CA)	19.12	0.44	0.44
25	assign (segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 393 and name CA)	16.97	0.50	0.49
	assign (segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 394 and name CA)	14.12	0.52	0.52
	assign (segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 394 and name CB)	14.22	0.61	0.61
	assign (segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 395 and name CA)	15.54	0.60	0.60
	assign (segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 396 and name CA)	16.03	0.55	0.54
30	assign (segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 396 and name CB)	17.03	0.56	0.57
	assign (segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 397 and name CA)	12.59	0.57	0.56
	assign (segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 397 and name CB)	12.04	0.58	0.58
	assign (segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 398 and name CA)	11.08	0.55	0.54
	assign (segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 398 and name CB)	11.30	0.57	0.57
35	assign (segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 399 and name CA)	13.98	0.50	0.50
	assign (segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 399 and name CB)	15.41	0.50	0.49
	assign (segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 400 and name CA)	13.66	0.52	0.52
	assign (segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 400 and name CB)	13.88	0.47	0.47
	assign (segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 401 and name CA)	10.09	0.53	0.54
40	assign (segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 402 and name CA)	11.25	0.46	0.46
	assign (segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 402 and name CB)	11.80	0.43	0.44
	assign (segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 403 and name CA)	14.56	0.48	0.49
	assign (segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 403 and name CB)	15.58	0.47	0.48
	assign (segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 404 and name CA)	13.61	0.62	0.63
45	assign (segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 404 and name CB)	12.96	0.76	0.75
	assign (segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 405 and name CA)	11.46	0.39	0.38
	assign (segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 405 and name CB)	10.07	0.40	0.40
	assign (segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 406 and name CA)	14.14	0.40	0.40
	assign (segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 407 and name CA)	16.83	0.36	0.36
50	assign (segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 407 and name CB)	17.39	0.42	0.42
	assign (segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 408 and name CA)	15.80	0.27	0.27
	assign (segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 408 and name CB)	14.65	0.31	0.31
	assign (segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 409 and name CA)	15.51	0.50	0.51
	assign (segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 409 and name CB)	14.47	0.56	0.55
55	assign (segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 410 and name CA)	18.64	0.40	0.40
	assign (segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 414 and name CA)	17.61	0.82	0.83
	assign (segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 415 and name CA)	18.14	0.76	0.76
	assign (segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 425 and name CA)	16.33	1.77	1.78
	assign (segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 426 and name CA)	15.62	1.40	1.39
60	assign (segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 427 and name CA)	16.17	0.98	0.97
	assign (segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 428 and name CA)	18.15	1.17	1.18
	assign (segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 429 and name CA)	18.25	0.69	0.70
	assign (segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 431 and name CA)	17.99	0.39	0.40
	assign (segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 433 and name CA)	13.06	0.76	0.75
65	assign (segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 434 and name CA)	12.50	0.99	0.99
	assign (segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 435 and name CA)	13.20	1.07	1.08
	assign (segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 436 and name CA)	16.65	1.19	1.20
	assign (segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 437 and name CA)	17.82	0.88	0.87
	assign (segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 438 and name CA)	16.34	0.95	0.94
70	assign (segid 3A4 and resid 312 and name CA)	(segid 3A4 and resid 440 and name CA)	18.58	0.76	0.76
	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 313 and name C)	5.45	0.05	0.05
	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 313 and name CA)	4.50	0.07	0.06
	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 313 and name CB)	5.33	0.10	0.10
	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 313 and name CG)	5.26	0.26	0.26
75	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 313 and name H)	3.16	0.06	0.07
	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 313 and name O)	6.41	0.08	0.09
	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 314 and name C)	6.89	0.08	0.08
	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 314 and name CA)	6.78	0.05	0.05
	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 314 and name CB)	7.27	0.08	0.07
80	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 314 and name N)	5.57	0.05	0.05
	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 315 and name C)	6.77	0.16	0.15
	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 315 and name CA)	6.55	0.13	0.12
	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 315 and name CB)	6.01	0.11	0.10

	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 315 and name N)	6.06	0.11	0.11
	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 316 and name C)	7.16	0.36	0.35
	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 316 and name CA)	6.62	0.24	0.24
	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 316 and name N)	5.95	0.17	0.16
5	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 317 and name CA)	8.64	0.36	0.35
	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 318 and name CA)	10.09	0.52	0.52
	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 318 and name CB)	9.61	0.49	0.49
	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 319 and name CA)	13.27	0.49	0.49
	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 319 and name CB)	13.58	0.41	0.41
10	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 346 and name CA)	17.94	0.48	0.48
	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 346 and name CB)	18.39	0.51	0.51
	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 347 and name CA)	14.83	0.46	0.46
	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 347 and name CB)	14.21	0.50	0.51
	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 348 and name CA)	13.03	0.60	0.60
15	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 349 and name CA)	15.81	0.63	0.64
	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 349 and name CB)	17.24	0.63	0.62
	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 350 and name CA)	15.66	0.27	0.27
	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 350 and name CB)	15.78	0.32	0.32
	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 351 and name CA)	12.22	0.18	0.18
20	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 352 and name CA)	13.66	0.40	0.39
	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 352 and name CB)	13.72	0.39	0.39
	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 353 and name CA)	16.95	0.39	0.38
	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 353 and name CB)	17.46	0.37	0.37
	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 354 and name CA)	18.39	0.51	0.50
25	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 356 and name CA)	17.68	0.46	0.47
	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 356 and name CB)	17.06	0.46	0.47
	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 357 and name CA)	15.10	0.46	0.45
	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 357 and name CB)	13.73	0.50	0.50
	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 358 and name CA)	17.13	0.55	0.55
30	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 358 and name CB)	17.90	0.80	0.80
	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 359 and name CA)	15.82	0.33	0.33
	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 359 and name CB)	15.90	0.34	0.34
	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 360 and name CA)	13.30	0.29	0.29
	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 360 and name CB)	14.08	0.31	0.31
35	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 361 and name CA)	12.74	0.43	0.44
	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 361 and name CB)	13.95	0.49	0.50
	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 362 and name CA)	11.80	0.32	0.33
	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 362 and name CB)	12.87	0.25	0.24
	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 363 and name CA)	8.50	0.22	0.22
40	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 363 and name CB)	7.86	0.33	0.33
	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 363 and name CG)	6.65	0.26	0.25
	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 364 and name CA)	9.74	0.14	0.15
	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 364 and name CB)	11.07	0.14	0.14
	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 365 and name CA)	8.61	0.17	0.17
45	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 365 and name CB)	8.53	0.23	0.22
	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 381 and name CA)	11.94	0.39	0.39
	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 382 and name CA)	13.26	0.27	0.26
	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 382 and name CB)	14.52	0.33	0.32
	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 383 and name CA)	10.60	0.31	0.32
50	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 384 and name CA)	12.88	0.42	0.42
	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 384 and name CB)	12.86	0.47	0.47
	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 385 and name CA)	15.95	0.36	0.35
	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 386 and name CA)	18.66	0.42	0.41
	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 390 and name CA)	18.67	0.41	0.41
55	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 390 and name CB)	18.65	0.41	0.41
	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 391 and name CA)	16.80	0.46	0.47
	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 391 and name CB)	15.32	0.46	0.46
	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 392 and name CA)	18.99	0.47	0.48
	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 393 and name CA)	16.59	0.54	0.53
60	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 394 and name CA)	13.89	0.55	0.55
	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 394 and name CB)	14.14	0.61	0.61
	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 395 and name CA)	15.10	0.62	0.62
	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 396 and name CA)	15.29	0.59	0.58
	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 396 and name CB)	16.29	0.59	0.60
65	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 397 and name CA)	11.84	0.60	0.60
	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 397 and name CB)	11.43	0.61	0.61
	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 398 and name CA)	10.37	0.57	0.58
	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 398 and name CB)	10.76	0.60	0.59
	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 399 and name CA)	13.04	0.55	0.54
70	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 399 and name CB)	14.48	0.54	0.54
	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 400 and name CA)	12.47	0.55	0.56
	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 400 and name CB)	12.72	0.51	0.50
	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 401 and name CA)	8.83	0.58	0.58
	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 402 and name CA)	10.08	0.50	0.50
75	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 402 and name CB)	10.77	0.47	0.47
	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 403 and name CA)	13.26	0.53	0.52
	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 403 and name CB)	14.28	0.51	0.52
	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 404 and name CA)	12.15	0.65	0.65
	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 404 and name CB)	11.49	0.78	0.78
80	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 405 and name CA)	10.02	0.40	0.40
	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 405 and name CB)	8.67	0.43	0.43
	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 406 and name CA)	12.83	0.43	0.44
	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 407 and name CA)	15.41	0.39	0.39

	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 407 and name CB)	15.95	0.45	0.44
	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 408 and name CA)	14.34	0.26	0.27
	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 408 and name CB)	13.19	0.29	0.29
	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 409 and name CA)	14.21	0.49	0.49
	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 409 and name CB)	13.23	0.56	0.56
5	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 410 and name CA)	17.36	0.40	0.40
	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 411 and name CA)	19.10	0.41	0.41
	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 412 and name CA)	18.19	0.53	0.54
	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 414 and name CA)	16.55	0.73	0.72
	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 415 and name CA)	17.25	0.59	0.60
10	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 415 and name CB)	18.27	0.82	0.82
	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 425 and name CA)	16.16	1.60	1.61
	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 426 and name CA)	15.56	1.23	1.23
	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 427 and name CA)	16.13	1.01	1.02
	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 429 and name CA)	18.44	0.83	0.82
15	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 431 and name CA)	18.24	0.43	0.43
	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 433 and name CA)	13.15	0.79	0.80
	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 434 and name CA)	12.26	0.96	0.97
	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 435 and name CA)	12.77	1.01	1.01
	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 436 and name CA)	16.11	1.12	1.12
20	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 437 and name CA)	17.09	0.77	0.76
	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 438 and name CA)	15.50	0.86	0.87
	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 439 and name CA)	18.10	0.81	0.81
	assign (segid 3A4 and resid 312 and name CB)	(segid 3A4 and resid 440 and name CA)	17.53	0.67	0.67
	assign (segid 3A4 and resid 312 and name N)	(segid 3A4 and resid 312 and name C)	2.45	0.02	0.02
25	assign (segid 3A4 and resid 312 and name N)	(segid 3A4 and resid 312 and name CA)	1.45	0.02	0.02
	assign (segid 3A4 and resid 312 and name N)	(segid 3A4 and resid 312 and name CB)	2.45	0.02	0.02
	assign (segid 3A4 and resid 312 and name N)	(segid 3A4 and resid 312 and name O)	3.48	0.04	0.04
	assign (segid 3A4 and resid 312 and name N)	(segid 3A4 and resid 313 and name C)	4.66	0.05	0.05
	assign (segid 3A4 and resid 312 and name N)	(segid 3A4 and resid 313 and name CA)	4.21	0.04	0.04
30	assign (segid 3A4 and resid 312 and name N)	(segid 3A4 and resid 313 and name CB)	4.99	0.06	0.05
	assign (segid 3A4 and resid 312 and name N)	(segid 3A4 and resid 313 and name CG)	5.48	0.12	0.12
	assign (segid 3A4 and resid 312 and name N)	(segid 3A4 and resid 313 and name N)	2.81	0.04	0.03
	assign (segid 3A4 and resid 312 and name N)	(segid 3A4 and resid 313 and name O)	5.81	0.08	0.07
	assign (segid 3A4 and resid 312 and name N)	(segid 3A4 and resid 314 and name C)	5.57	0.07	0.07
35	assign (segid 3A4 and resid 312 and name N)	(segid 3A4 and resid 314 and name CA)	5.24	0.05	0.05
	assign (segid 3A4 and resid 312 and name N)	(segid 3A4 and resid 314 and name CB)	5.31	0.08	0.08
	assign (segid 3A4 and resid 312 and name N)	(segid 3A4 and resid 314 and name CG)	6.69	0.11	0.11
	assign (segid 3A4 and resid 312 and name N)	(segid 3A4 and resid 314 and name N)	4.21	0.03	0.04
	assign (segid 3A4 and resid 312 and name N)	(segid 3A4 and resid 314 and name O)	6.74	0.06	0.06
40	assign (segid 3A4 and resid 312 and name N)	(segid 3A4 and resid 315 and name C)	6.29	0.13	0.12
	assign (segid 3A4 and resid 312 and name N)	(segid 3A4 and resid 315 and name CA)	5.57	0.13	0.13
	assign (segid 3A4 and resid 312 and name N)	(segid 3A4 and resid 315 and name CB)	5.08	0.19	0.19
	assign (segid 3A4 and resid 312 and name N)	(segid 3A4 and resid 315 and name N)	4.78	0.11	0.10
	assign (segid 3A4 and resid 312 and name N)	(segid 3A4 and resid 315 and name O)	7.50	0.12	0.12
45	assign (segid 3A4 and resid 312 and name N)	(segid 3A4 and resid 316 and name C)	6.95	0.19	0.19
	assign (segid 3A4 and resid 312 and name N)	(segid 3A4 and resid 316 and name N)	5.85	0.15	0.15
	assign (segid 3A4 and resid 312 and name N)	(segid 3A4 and resid 363 and name C)	7.69	0.07	0.07
	assign (segid 3A4 and resid 312 and name N)	(segid 3A4 and resid 363 and name CA)	7.28	0.13	0.14
	assign (segid 3A4 and resid 312 and name N)	(segid 3A4 and resid 363 and name CB)	7.05	0.22	0.23
50	assign (segid 3A4 and resid 312 and name N)	(segid 3A4 and resid 363 and name CG)	5.95	0.20	0.21
	assign (segid 3A4 and resid 312 and name N)	(segid 3A4 and resid 364 and name C)	7.36	0.13	0.12
	assign (segid 3A4 and resid 312 and name N)	(segid 3A4 and resid 364 and name N)	7.33	0.11	0.12
	assign (segid 3A4 and resid 312 and name N)	(segid 3A4 and resid 364 and name O)	7.22	0.20	0.21
	assign (segid 3A4 and resid 312 and name N)	(segid 3A4 and resid 365 and name CA)	6.98	0.13	0.13
55	assign (segid 3A4 and resid 312 and name N)	(segid 3A4 and resid 365 and name CB)	7.26	0.14	0.14
	assign (segid 3A4 and resid 312 and name N)	(segid 3A4 and resid 365 and name N)	7.27	0.09	0.08
	assign (segid 3A4 and resid 312 and name O)	(segid 3A4 and resid 312 and name CB)	3.28	0.06	0.05
	assign (segid 3A4 and resid 312 and name O)	(segid 3A4 and resid 313 and name C)	3.06	0.07	0.07
	assign (segid 3A4 and resid 312 and name O)	(segid 3A4 and resid 313 and name CA)	2.77	0.06	0.05
60	assign (segid 3A4 and resid 312 and name O)	(segid 3A4 and resid 313 and name CB)	4.25	0.06	0.05
	assign (segid 3A4 and resid 312 and name O)	(segid 3A4 and resid 313 and name CG)	4.90	0.13	0.13
	assign (segid 3A4 and resid 312 and name O)	(segid 3A4 and resid 313 and name N)	2.25	0.03	0.03
	assign (segid 3A4 and resid 312 and name O)	(segid 3A4 and resid 313 and name O)	3.66	0.15	0.15
	assign (segid 3A4 and resid 312 and name O)	(segid 3A4 and resid 314 and name C)	4.16	0.05	0.05
65	assign (segid 3A4 and resid 312 and name O)	(segid 3A4 and resid 314 and name CA)	4.42	0.05	0.05
	assign (segid 3A4 and resid 312 and name O)	(segid 3A4 and resid 314 and name CB)	5.41	0.05	0.05
	assign (segid 3A4 and resid 312 and name O)	(segid 3A4 and resid 314 and name CG)	6.65	0.08	0.07
	assign (segid 3A4 and resid 312 and name O)	(segid 3A4 and resid 314 and name N)	3.45	0.05	0.06
	assign (segid 3A4 and resid 312 and name O)	(segid 3A4 and resid 314 and name O)	4.94	0.07	0.07
70	assign (segid 3A4 and resid 312 and name O)	(segid 3A4 and resid 315 and name C)	3.88	0.06	0.05
	assign (segid 3A4 and resid 312 and name O)	(segid 3A4 and resid 315 and name CA)	4.00	0.07	0.06
	assign (segid 3A4 and resid 312 and name O)	(segid 3A4 and resid 315 and name CB)	4.13	0.12	0.12
	assign (segid 3A4 and resid 312 and name O)	(segid 3A4 and resid 315 and name N)	3.52	0.07	0.07
	assign (segid 3A4 and resid 312 and name O)	(segid 3A4 and resid 315 and name O)	5.04	0.07	0.07
75	assign (segid 3A4 and resid 312 and name O)	(segid 3A4 and resid 316 and name C)	4.09	0.32	0.31
	assign (segid 3A4 and resid 312 and name O)	(segid 3A4 and resid 316 and name CA)	3.67	0.16	0.16
	assign (segid 3A4 and resid 312 and name O)	(segid 3A4 and resid 316 and name N)	2.91	0.10	0.10
	assign (segid 3A4 and resid 312 and name O)	(segid 3A4 and resid 316 and name O)	4.45	0.81	0.81
80	assign (segid 3A4 and resid 312 and name O)	(segid 3A4 and resid 317 and name C)	6.47	0.21	0.21
	assign (segid 3A4 and resid 312 and name O)	(segid 3A4 and resid 317 and name CA)	5.56	0.25	0.26
	assign (segid 3A4 and resid 312 and name O)	(segid 3A4 and resid 317 and name N)	4.58	0.16	0.17
	assign (segid 3A4 and resid 312 and name O)	(segid 3A4 and resid 317 and name O)	7.35	0.31	0.31

	assign (segid 3A4 and resid 312 and name O)	(segid 3A4 and resid 318 and name N)	6.58	0.35	0.35
	assign (segid 3A4 and resid 312 and name O)	(segid 3A4 and resid 363 and name CG)	7.37	0.25	0.24
	assign (segid 3A4 and resid 313 and name C)	(segid 3A4 and resid 313 and name CB)	2.49	0.01	0.02
	assign (segid 3A4 and resid 313 and name C)	(segid 3A4 and resid 313 and name CG)	3.91	0.09	0.09
5	assign (segid 3A4 and resid 313 and name C)	(segid 3A4 and resid 313 and name O)	1.21	0.02	0.02
	assign (segid 3A4 and resid 313 and name C)	(segid 3A4 and resid 314 and name C)	3.08	0.06	0.06
	assign (segid 3A4 and resid 313 and name C)	(segid 3A4 and resid 314 and name CA)	2.44	0.02	0.02
	assign (segid 3A4 and resid 313 and name C)	(segid 3A4 and resid 314 and name CB)	3.72	0.03	0.04
	assign (segid 3A4 and resid 313 and name C)	(segid 3A4 and resid 314 and name CG)	4.98	0.04	0.03
10	assign (segid 3A4 and resid 313 and name C)	(segid 3A4 and resid 314 and name N)	1.34	0.02	0.01
	assign (segid 3A4 and resid 313 and name C)	(segid 3A4 and resid 314 and name O)	3.79	0.08	0.08
	assign (segid 3A4 and resid 313 and name C)	(segid 3A4 and resid 315 and name C)	4.83	0.13	0.13
	assign (segid 3A4 and resid 313 and name C)	(segid 3A4 and resid 315 and name CA)	4.69	0.12	0.12
	assign (segid 3A4 and resid 313 and name C)	(segid 3A4 and resid 315 and name CB)	5.54	0.15	0.15
15	assign (segid 3A4 and resid 313 and name C)	(segid 3A4 and resid 315 and name N)	3.50	0.12	0.11
	assign (segid 3A4 and resid 313 and name C)	(segid 3A4 and resid 315 and name O)	5.85	0.15	0.16
	assign (segid 3A4 and resid 313 and name C)	(segid 3A4 and resid 316 and name C)	4.69	0.23	0.24
	assign (segid 3A4 and resid 313 and name C)	(segid 3A4 and resid 316 and name CA)	5.01	0.11	0.10
	assign (segid 3A4 and resid 313 and name C)	(segid 3A4 and resid 316 and name N)	4.24	0.12	0.12
20	assign (segid 3A4 and resid 313 and name C)	(segid 3A4 and resid 316 and name O)	5.18	0.70	0.69
	assign (segid 3A4 and resid 313 and name C)	(segid 3A4 and resid 317 and name C)	6.00	0.20	0.19
	assign (segid 3A4 and resid 313 and name C)	(segid 3A4 and resid 317 and name CA)	4.74	0.26	0.26
	assign (segid 3A4 and resid 313 and name C)	(segid 3A4 and resid 317 and name N)	4.37	0.26	0.25
	assign (segid 3A4 and resid 313 and name C)	(segid 3A4 and resid 317 and name O)	7.03	0.25	0.25
25	assign (segid 3A4 and resid 313 and name C)	(segid 3A4 and resid 318 and name N)	6.18	0.27	0.28
	assign (segid 3A4 and resid 313 and name C)	(segid 3A4 and resid 351 and name CA)	7.49	0.18	0.18
	assign (segid 3A4 and resid 313 and name C)	(segid 3A4 and resid 381 and name CA)	7.22	0.39	0.39
	assign (segid 3A4 and resid 313 and name C)	(segid 3A4 and resid 382 and name C)	7.27	0.33	0.32
	assign (segid 3A4 and resid 313 and name C)	(segid 3A4 and resid 382 and name N)	7.37	0.31	0.31
30	assign (segid 3A4 and resid 313 and name C)	(segid 3A4 and resid 383 and name C)	6.69	0.43	0.42
	assign (segid 3A4 and resid 313 and name C)	(segid 3A4 and resid 383 and name CA)	5.60	0.39	0.39
	assign (segid 3A4 and resid 313 and name C)	(segid 3A4 and resid 383 and name N)	6.08	0.37	0.36
	assign (segid 3A4 and resid 313 and name C)	(segid 3A4 and resid 383 and name O)	7.08	0.40	0.39
	assign (segid 3A4 and resid 313 and name C)	(segid HEM and resid 1 and name CMB)	7.24	0.45	0.45
35	assign (segid 3A4 and resid 313 and name CA)	(segid 3A4 and resid 313 and name C)	1.52	0.00	0.01
	assign (segid 3A4 and resid 313 and name CA)	(segid 3A4 and resid 313 and name CB)	1.53	0.01	0.00
	assign (segid 3A4 and resid 313 and name CA)	(segid 3A4 and resid 313 and name CG)	2.60	0.09	0.09
	assign (segid 3A4 and resid 313 and name CA)	(segid 3A4 and resid 313 and name O)	2.38	0.02	0.02
	assign (segid 3A4 and resid 313 and name CA)	(segid 3A4 and resid 314 and name C)	4.44	0.04	0.04
40	assign (segid 3A4 and resid 313 and name CA)	(segid 3A4 and resid 314 and name CA)	3.84	0.04	0.03
	assign (segid 3A4 and resid 313 and name CA)	(segid 3A4 and resid 314 and name CB)	4.92	0.06	0.07
	assign (segid 3A4 and resid 313 and name CA)	(segid 3A4 and resid 314 and name CG)	6.30	0.06	0.07
	assign (segid 3A4 and resid 313 and name CA)	(segid 3A4 and resid 314 and name N)	2.47	0.04	0.04
	assign (segid 3A4 and resid 313 and name CA)	(segid 3A4 and resid 314 and name O)	5.21	0.08	0.07
45	assign (segid 3A4 and resid 313 and name CA)	(segid 3A4 and resid 315 and name C)	5.67	0.10	0.09
	assign (segid 3A4 and resid 313 and name CA)	(segid 3A4 and resid 315 and name CA)	5.63	0.08	0.08
	assign (segid 3A4 and resid 313 and name CA)	(segid 3A4 and resid 315 and name CB)	6.21	0.12	0.12
	assign (segid 3A4 and resid 313 and name CA)	(segid 3A4 and resid 315 and name N)	4.56	0.07	0.08
	assign (segid 3A4 and resid 313 and name CA)	(segid 3A4 and resid 315 and name O)	6.76	0.11	0.11
50	assign (segid 3A4 and resid 313 and name CA)	(segid 3A4 and resid 316 and name C)	5.09	0.34	0.35
	assign (segid 3A4 and resid 313 and name CA)	(segid 3A4 and resid 316 and name CA)	5.40	0.13	0.14
	assign (segid 3A4 and resid 313 and name CA)	(segid 3A4 and resid 316 and name N)	4.81	0.11	0.12
	assign (segid 3A4 and resid 313 and name CA)	(segid 3A4 and resid 316 and name O)	5.34	0.90	0.90
	assign (segid 3A4 and resid 313 and name CA)	(segid 3A4 and resid 317 and name C)	6.39	0.38	0.38
55	assign (segid 3A4 and resid 313 and name CA)	(segid 3A4 and resid 317 and name CA)	5.37	0.46	0.45
	assign (segid 3A4 and resid 313 and name CA)	(segid 3A4 and resid 317 and name N)	5.03	0.30	0.30
	assign (segid 3A4 and resid 313 and name CA)	(segid 3A4 and resid 318 and name CA)	7.49	0.43	0.43
	assign (segid 3A4 and resid 313 and name CA)	(segid 3A4 and resid 318 and name CB)	7.32	0.46	0.45
	assign (segid 3A4 and resid 313 and name CA)	(segid 3A4 and resid 318 and name N)	6.30	0.43	0.42
60	assign (segid 3A4 and resid 313 and name CA)	(segid 3A4 and resid 319 and name CA)	9.83	0.40	0.41
	assign (segid 3A4 and resid 313 and name CA)	(segid 3A4 and resid 319 and name CB)	9.95	0.33	0.32
	assign (segid 3A4 and resid 313 and name CA)	(segid 3A4 and resid 322 and name CA)	19.38	0.42	0.41
	assign (segid 3A4 and resid 313 and name CA)	(segid 3A4 and resid 344 and name CA)	19.29	0.43	0.43
	assign (segid 3A4 and resid 313 and name CA)	(segid 3A4 and resid 344 and name CB)	19.42	0.37	0.38
65	assign (segid 3A4 and resid 313 and name CA)	(segid 3A4 and resid 345 and name CA)	16.46	0.57	0.57
	assign (segid 3A4 and resid 313 and name CA)	(segid 3A4 and resid 345 and name CB)	16.25	0.80	0.79
	assign (segid 3A4 and resid 313 and name CA)	(segid 3A4 and resid 346 and name CA)	14.08	0.44	0.43
	assign (segid 3A4 and resid 313 and name CA)	(segid 3A4 and resid 346 and name CB)	14.72	0.44	0.44
	assign (segid 3A4 and resid 313 and name CA)	(segid 3A4 and resid 347 and name CA)	10.71	0.43	0.43
70	assign (segid 3A4 and resid 313 and name CA)	(segid 3A4 and resid 347 and name CB)	9.97	0.47	0.47
	assign (segid 3A4 and resid 313 and name CA)	(segid 3A4 and resid 348 and name CA)	9.61	0.54	0.54
	assign (segid 3A4 and resid 313 and name CA)	(segid 3A4 and resid 349 and name CA)	12.60	0.56	0.55
	assign (segid 3A4 and resid 313 and name CA)	(segid 3A4 and resid 349 and name CB)	13.97	0.51	0.51
	assign (segid 3A4 and resid 313 and name CA)	(segid 3A4 and resid 350 and name CA)	12.05	0.27	0.26
75	assign (segid 3A4 and resid 313 and name CA)	(segid 3A4 and resid 350 and name CB)	11.91	0.33	0.33
	assign (segid 3A4 and resid 313 and name CA)	(segid 3A4 and resid 351 and name CA)	8.99	0.19	0.19
	assign (segid 3A4 and resid 313 and name CA)	(segid 3A4 and resid 352 and name CA)	11.35	0.37	0.36
	assign (segid 3A4 and resid 313 and name CA)	(segid 3A4 and resid 352 and name CB)	11.55	0.38	0.39
	assign (segid 3A4 and resid 313 and name CA)	(segid 3A4 and resid 353 and name CA)	14.36	0.32	0.32
80	assign (segid 3A4 and resid 313 and name CA)	(segid 3A4 and resid 353 and name CB)	14.59	0.31	0.30
	assign (segid 3A4 and resid 313 and name CA)	(segid 3A4 and resid 354 and name CA)	16.52	0.39	0.40
	assign (segid 3A4 and resid 313 and name CA)	(segid 3A4 and resid 354 and name CB)	17.67	0.45	0.45
	assign (segid 3A4 and resid 313 and name CA)	(segid 3A4 and resid 355 and name CA)	18.21	0.32	0.33

assign (segid 3A4 and resid 313 and name CA) (segid 3A4 and resid 355 and name CB) 18.95 0.29 0.29
 assign (segid 3A4 and resid 313 and name CA) (segid 3A4 and resid 356 and name CA) 15.29 0.38 0.38
 assign (segid 3A4 and resid 313 and name CA) (segid 3A4 and resid 356 and name CB) 14.37 0.39 0.39
 assign (segid 3A4 and resid 313 and name CA) (segid 3A4 and resid 357 and name CA) 13.49 0.36 0.35
 assign (segid 3A4 and resid 313 and name CA) (segid 3A4 and resid 357 and name CB) 12.07 0.41 0.41
 5 assign (segid 3A4 and resid 313 and name CA) (segid 3A4 and resid 358 and name CA) 16.37 0.54 0.54
 assign (segid 3A4 and resid 313 and name CA) (segid 3A4 and resid 358 and name CB) 17.33 0.76 0.76
 assign (segid 3A4 and resid 313 and name CA) (segid 3A4 and resid 359 and name CA) 15.70 0.19 0.18
 assign (segid 3A4 and resid 313 and name CA) (segid 3A4 and resid 359 and name CB) 16.15 0.17 0.16
 10 assign (segid 3A4 and resid 313 and name CA) (segid 3A4 and resid 360 and name CA) 12.50 0.19 0.20
 assign (segid 3A4 and resid 313 and name CA) (segid 3A4 and resid 360 and name CB) 12.84 0.26 0.26
 assign (segid 3A4 and resid 313 and name CA) (segid 3A4 and resid 361 and name CA) 12.75 0.22 0.21
 assign (segid 3A4 and resid 313 and name CA) (segid 3A4 and resid 361 and name CB) 13.97 0.24 0.23
 assign (segid 3A4 and resid 313 and name CA) (segid 3A4 and resid 362 and name CA) 12.91 0.18 0.18
 assign (segid 3A4 and resid 313 and name CA) (segid 3A4 and resid 362 and name CB) 14.03 0.15 0.14
 15 assign (segid 3A4 and resid 313 and name CA) (segid 3A4 and resid 363 and name CA) 10.47 0.13 0.13
 assign (segid 3A4 and resid 313 and name CA) (segid 3A4 and resid 363 and name CB) 10.31 0.18 0.18
 assign (segid 3A4 and resid 313 and name CA) (segid 3A4 and resid 364 and name CA) 11.74 0.09 0.10
 assign (segid 3A4 and resid 313 and name CA) (segid 3A4 and resid 364 and name CB) 12.73 0.09 0.09
 20 assign (segid 3A4 and resid 313 and name CA) (segid 3A4 and resid 365 and name CA) 10.88 0.17 0.18
 assign (segid 3A4 and resid 313 and name CA) (segid 3A4 and resid 365 and name CB) 11.29 0.16 0.17
 assign (segid 3A4 and resid 313 and name CA) (segid 3A4 and resid 381 and name CA) 8.26 0.30 0.31
 assign (segid 3A4 and resid 313 and name CA) (segid 3A4 and resid 382 and name CA) 8.92 0.24 0.23
 assign (segid 3A4 and resid 313 and name CA) (segid 3A4 and resid 382 and name CB) 10.17 0.28 0.27
 assign (segid 3A4 and resid 313 and name CA) (segid 3A4 and resid 383 and name C) 6.97 0.34 0.33
 25 assign (segid 3A4 and resid 313 and name CA) (segid 3A4 and resid 383 and name CA) 6.14 0.29 0.30
 assign (segid 3A4 and resid 313 and name CA) (segid 3A4 and resid 383 and name N) 6.79 0.25 0.25
 assign (segid 3A4 and resid 313 and name CA) (segid 3A4 and resid 383 and name O) 7.24 0.33 0.33
 assign (segid 3A4 and resid 313 and name CA) (segid 3A4 and resid 384 and name CA) 8.70 0.40 0.41
 assign (segid 3A4 and resid 313 and name CA) (segid 3A4 and resid 384 and name CB) 8.90 0.46 0.47
 30 assign (segid 3A4 and resid 313 and name CA) (segid 3A4 and resid 385 and name CA) 11.54 0.32 0.32
 assign (segid 3A4 and resid 313 and name CA) (segid 3A4 and resid 386 and name CA) 14.31 0.37 0.37
 assign (segid 3A4 and resid 313 and name CA) (segid 3A4 and resid 387 and name CA) 17.77 0.26 0.27
 assign (segid 3A4 and resid 313 and name CA) (segid 3A4 and resid 389 and name CA) 17.83 0.47 0.47
 assign (segid 3A4 and resid 313 and name CA) (segid 3A4 and resid 389 and name CB) 18.06 0.56 0.55
 35 assign (segid 3A4 and resid 313 and name CA) (segid 3A4 and resid 390 and name CA) 14.59 0.39 0.39
 assign (segid 3A4 and resid 313 and name CA) (segid 3A4 and resid 390 and name CB) 14.61 0.38 0.38
 assign (segid 3A4 and resid 313 and name CA) (segid 3A4 and resid 391 and name CA) 13.12 0.42 0.43
 assign (segid 3A4 and resid 313 and name CA) (segid 3A4 and resid 391 and name CB) 11.70 0.43 0.42
 40 assign (segid 3A4 and resid 313 and name CA) (segid 3A4 and resid 392 and name CA) 15.80 0.45 0.45
 assign (segid 3A4 and resid 313 and name CA) (segid 3A4 and resid 392 and name CB) 17.09 0.49 0.49
 assign (segid 3A4 and resid 313 and name CA) (segid 3A4 and resid 393 and name CA) 14.03 0.51 0.51
 assign (segid 3A4 and resid 313 and name CA) (segid 3A4 and resid 394 and name CA) 11.20 0.55 0.54
 assign (segid 3A4 and resid 313 and name CA) (segid 3A4 and resid 394 and name CB) 11.17 0.65 0.64
 45 assign (segid 3A4 and resid 313 and name CA) (segid 3A4 and resid 395 and name CA) 13.29 0.62 0.62
 assign (segid 3A4 and resid 313 and name CA) (segid 3A4 and resid 396 and name CA) 14.06 0.56 0.57
 assign (segid 3A4 and resid 313 and name CA) (segid 3A4 and resid 396 and name CB) 14.94 0.59 0.59
 assign (segid 3A4 and resid 313 and name CA) (segid 3A4 and resid 397 and name CA) 10.62 0.58 0.57
 assign (segid 3A4 and resid 313 and name CA) (segid 3A4 and resid 397 and name CB) 9.71 0.60 0.60
 50 assign (segid 3A4 and resid 313 and name CA) (segid 3A4 and resid 397 and name CB) 9.70 0.54 0.55
 assign (segid 3A4 and resid 313 and name CA) (segid 3A4 and resid 398 and name CA) 9.79 0.58 0.58
 assign (segid 3A4 and resid 313 and name CA) (segid 3A4 and resid 398 and name CB) 13.18 0.53 0.53
 assign (segid 3A4 and resid 313 and name CA) (segid 3A4 and resid 399 and name CA) 14.43 0.52 0.52
 assign (segid 3A4 and resid 313 and name CA) (segid 3A4 and resid 399 and name CB) 13.12 0.54 0.54
 55 assign (segid 3A4 and resid 313 and name CA) (segid 3A4 and resid 400 and name CA) 13.07 0.51 0.50
 assign (segid 3A4 and resid 313 and name CA) (segid 3A4 and resid 400 and name CB) 10.17 0.54 0.54
 assign (segid 3A4 and resid 313 and name CA) (segid 3A4 and resid 401 and name CA) 11.91 0.45 0.46
 assign (segid 3A4 and resid 313 and name CA) (segid 3A4 and resid 402 and name CA) 12.24 0.46 0.45
 assign (segid 3A4 and resid 313 and name CA) (segid 3A4 and resid 402 and name CB) 15.25 0.49 0.50
 60 assign (segid 3A4 and resid 313 and name CA) (segid 3A4 and resid 403 and name CA) 15.97 0.48 0.49
 assign (segid 3A4 and resid 313 and name CA) (segid 3A4 and resid 403 and name CB) 14.67 0.57 0.57
 assign (segid 3A4 and resid 313 and name CA) (segid 3A4 and resid 404 and name CA) 13.85 0.68 0.68
 assign (segid 3A4 and resid 313 and name CA) (segid 3A4 and resid 404 and name CB) 13.35 0.38 0.38
 assign (segid 3A4 and resid 313 and name CA) (segid 3A4 and resid 405 and name CA) 12.04 0.39 0.39
 assign (segid 3A4 and resid 313 and name CA) (segid 3A4 and resid 405 and name CB) 16.06 0.44 0.44
 65 assign (segid 3A4 and resid 313 and name CA) (segid 3A4 and resid 406 and name CA) 18.64 0.39 0.40
 assign (segid 3A4 and resid 313 and name CA) (segid 3A4 and resid 407 and name CA) 17.99 0.24 0.25
 assign (segid 3A4 and resid 313 and name CA) (segid 3A4 and resid 408 and name CA) 16.84 0.24 0.24
 assign (segid 3A4 and resid 313 and name CA) (segid 3A4 and resid 409 and name CA) 18.28 0.49 0.49
 assign (segid 3A4 and resid 313 and name CA) (segid 3A4 and resid 409 and name CB) 17.33 0.57 0.57
 70 assign (segid 3A4 and resid 313 and name CA) (segid 3A4 and resid 425 and name CA) 17.52 1.64 1.64
 assign (segid 3A4 and resid 313 and name CA) (segid 3A4 and resid 426 and name CA) 16.10 1.57 1.56
 assign (segid 3A4 and resid 313 and name CA) (segid 3A4 and resid 427 and name CA) 15.92 0.76 0.76
 assign (segid 3A4 and resid 313 and name CA) (segid 3A4 and resid 428 and name CA) 17.38 1.19 1.19
 75 assign (segid 3A4 and resid 313 and name CA) (segid 3A4 and resid 429 and name CA) 16.94 0.80 0.80
 assign (segid 3A4 and resid 313 and name CA) (segid 3A4 and resid 430 and name CA) 17.20 1.11 1.12
 assign (segid 3A4 and resid 313 and name CA) (segid 3A4 and resid 431 and name CA) 15.61 0.66 0.66
 assign (segid 3A4 and resid 313 and name CA) (segid 3A4 and resid 433 and name CA) 11.72 0.58 0.57
 assign (segid 3A4 and resid 313 and name CA) (segid 3A4 and resid 434 and name CA) 11.97 0.31 0.32
 80 assign (segid 3A4 and resid 313 and name CA) (segid 3A4 and resid 435 and name CA) 13.67 0.96 0.96
 assign (segid 3A4 and resid 313 and name CA) (segid 3A4 and resid 436 and name CA) 17.10 1.07 1.06
 assign (segid 3A4 and resid 313 and name CA) (segid 3A4 and resid 437 and name CA) 18.86 0.81 0.81
 assign (segid 3A4 and resid 313 and name CA) (segid 3A4 and resid 438 and name CA) 18.06 0.83 0.82

	assign (segid 3A4 and resid 313 and name CA)	(segid HEM and resid 1 and name CBB)	6.99	0.53	0.53
	assign (segid 3A4 and resid 313 and name CA)	(segid HEM and resid 1 and name CNB)	6.73	0.45	0.45
	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 313 and name CG)	1.56	0.08	0.09
	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 314 and name C)	5.52	0.07	0.06
5	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 314 and name CA)	4.58	0.06	0.05
	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 314 and name CB)	5.50	0.08	0.08
	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 314 and name CG)	6.87	0.08	0.08
	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 314 and name N)	3.27	0.06	0.05
	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 314 and name O)	6.25	0.10	0.09
10	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 315 and name C)	7.11	0.11	0.11
	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 315 and name CA)	7.01	0.09	0.09
	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 315 and name CB)	7.61	0.12	0.13
	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 315 and name N)	5.82	0.09	0.09
	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 316 and name C)	6.35	0.35	0.36
15	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 316 and name CA)	6.82	0.14	0.15
	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 316 and name N)	6.30	0.13	0.12
	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 317 and name C)	7.16	0.49	0.48
	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 317 and name CA)	6.20	0.54	0.54
	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 317 and name N)	6.14	0.35	0.35
20	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 318 and name CA)	8.07	0.53	0.53
	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 318 and name CB)	7.78	0.59	0.59
	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 319 and name CA)	10.01	0.48	0.48
	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 319 and name CB)	9.90	0.40	0.39
	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 322 and name CA)	19.20	0.43	0.44
25	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 345 and name CA)	16.49	0.59	0.60
	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 345 and name CB)	16.15	0.84	0.84
	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 346 and name CA)	14.40	0.40	0.39
	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 346 and name CB)	15.17	0.38	0.38
	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 347 and name CA)	10.88	0.40	0.40
30	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 347 and name CB)	10.02	0.45	0.44
	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 348 and name CA)	10.30	0.49	0.50
	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 349 and name CA)	13.27	0.49	0.49
	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 349 and name CB)	14.60	0.43	0.43
	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 350 and name CA)	12.36	0.26	0.26
35	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 350 and name CB)	12.05	0.34	0.35
	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 351 and name CA)	9.47	0.22	0.23
	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 352 and name CA)	12.19	0.37	0.36
	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 352 and name CB)	12.52	0.39	0.38
	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 353 and name CA)	14.94	0.31	0.31
40	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 353 and name CB)	15.03	0.30	0.31
	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 354 and name CA)	17.18	0.37	0.38
	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 354 and name CB)	18.40	0.42	0.42
	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 355 and name CA)	18.60	0.29	0.30
	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 355 and name CB)	19.29	0.26	0.26
45	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 356 and name CA)	15.50	0.36	0.36
	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 356 and name CB)	14.52	0.36	0.36
	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 357 and name CA)	13.94	0.33	0.32
	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 357 and name CB)	12.59	0.40	0.39
	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 358 and name CA)	17.05	0.58	0.58
50	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 359 and name CA)	16.65	0.18	0.17
	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 359 and name CB)	17.10	0.15	0.16
	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 360 and name CA)	13.49	0.19	0.18
	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 360 and name CB)	13.78	0.25	0.24
	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 361 and name CA)	14.02	0.21	0.20
55	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 361 and name CB)	15.27	0.23	0.23
	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 362 and name CA)	14.12	0.18	0.17
	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 362 and name CB)	15.16	0.13	0.14
	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 363 and name CA)	11.63	0.11	0.11
	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 363 and name CB)	11.53	0.18	0.17
60	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 364 and name CA)	12.54	0.08	0.07
	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 364 and name CB)	13.50	0.09	0.09
	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 365 and name CA)	11.31	0.20	0.19
	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 365 and name CB)	11.69	0.21	0.21
	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 381 and name CA)	7.84	0.21	0.21
65	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 382 and name C)	7.52	0.20	0.20
	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 382 and name CA)	8.36	0.17	0.17
	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 382 and name CB)	9.72	0.21	0.21
	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 383 and name C)	6.23	0.30	0.30
	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 383 and name CA)	5.60	0.25	0.24
70	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 383 and name N)	6.20	0.19	0.19
	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 383 and name O)	6.61	0.33	0.33
	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 384 and name CA)	7.67	0.39	0.39
	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 384 and name CB)	7.68	0.44	0.45
	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 384 and name CD1)	6.29	0.76	0.77
75	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 384 and name CG)	6.70	0.48	0.49
	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 384 and name N)	6.73	0.34	0.33
	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 385 and name CA)	10.73	0.30	0.31
	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 386 and name CA)	13.39	0.34	0.34
	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 387 and name CA)	16.77	0.26	0.25
80	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 388 and name CA)	18.74	0.31	0.32
	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 389 and name CA)	16.81	0.46	0.47
	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 389 and name CB)	17.14	0.55	0.56
	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 390 and name CA)	13.46	0.38	0.38

	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 390 and name CB)	13.41	0.36	0.37
	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 391 and name CA)	11.95	0.44	0.43
	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 391 and name CB)	10.53	0.44	0.44
	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 392 and name CA)	14.51	0.47	0.46
	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 392 and name CB)	15.84	0.51	0.50
5	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 393 and name CA)	12.77	0.52	0.52
	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 394 and name CA)	9.79	0.55	0.55
	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 394 and name CB)	9.72	0.64	0.65
	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 395 and name CA)	11.85	0.63	0.63
	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 396 and name CA)	12.82	0.57	0.56
10	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 396 and name CB)	13.73	0.59	0.59
	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 397 and name CA)	9.51	0.58	0.57
	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 397 and name CB)	8.58	0.60	0.61
	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 398 and name CA)	8.49	0.56	0.56
	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 398 and name CB)	8.47	0.59	0.59
15	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 399 and name CA)	12.08	0.54	0.55
	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 399 and name CB)	13.28	0.54	0.53
	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 400 and name CA)	12.31	0.52	0.53
	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 400 and name CB)	12.28	0.48	0.48
	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 401 and name CA)	9.60	0.52	0.52
20	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 402 and name CA)	11.27	0.47	0.46
	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 402 and name CB)	11.44	0.47	0.48
	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 403 and name CA)	14.64	0.49	0.50
	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 403 and name CB)	15.28	0.48	0.48
	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 404 and name CA)	14.38	0.53	0.54
25	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 404 and name CB)	13.60	0.62	0.62
	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 405 and name CA)	13.29	0.37	0.38
	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 405 and name CB)	12.00	0.39	0.39
	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 406 and name CA)	15.82	0.45	0.45
	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 407 and name CA)	18.46	0.40	0.40
30	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 407 and name CB)	18.69	0.42	0.42
	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 408 and name CA)	18.10	0.23	0.24
	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 408 and name CB)	17.02	0.21	0.21
	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 409 and name CA)	18.50	0.48	0.48
	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 409 and name CB)	17.56	0.57	0.58
35	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 427 and name CA)	17.01	0.72	0.72
	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 429 and name CA)	17.79	0.90	0.89
	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 431 and name CA)	16.01	0.81	0.82
	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 433 and name CA)	12.56	0.57	0.58
	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 434 and name CA)	12.90	0.90	0.90
40	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 435 and name CA)	14.73	0.92	0.92
	assign (segid 3A4 and resid 313 and name CB)	(segid 3A4 and resid 1 and name CAB)	7.32	0.50	0.51
	assign (segid 3A4 and resid 313 and name CB)	(segid HEM and resid 1 and name CBB)	6.34	0.60	0.60
	assign (segid 3A4 and resid 313 and name CB)	(segid HEM and resid 1 and name CMB)	6.14	0.49	0.50
	assign (segid 3A4 and resid 313 and name CB)	(segid HEM and resid 1 and name C)	6.95	0.13	0.12
45	assign (segid 3A4 and resid 313 and name CG)	(segid 3A4 and resid 314 and name CA)	6.09	0.11	0.11
	assign (segid 3A4 and resid 313 and name CG)	(segid 3A4 and resid 314 and name CB)	6.97	0.09	0.10
	assign (segid 3A4 and resid 313 and name CG)	(segid 3A4 and resid 314 and name N)	4.72	0.11	0.12
	assign (segid 3A4 and resid 313 and name CG)	(segid 3A4 and resid 314 and name O)	7.68	0.14	0.14
	assign (segid 3A4 and resid 313 and name CG)	(segid 3A4 and resid 315 and name N)	7.11	0.15	0.15
50	assign (segid 3A4 and resid 313 and name CG)	(segid 3A4 and resid 316 and name C)	7.11	0.40	0.41
	assign (segid 3A4 and resid 313 and name CG)	(segid 3A4 and resid 316 and name CA)	7.59	0.16	0.16
	assign (segid 3A4 and resid 313 and name CG)	(segid 3A4 and resid 316 and name N)	7.24	0.16	0.15
	assign (segid 3A4 and resid 313 and name CG)	(segid 3A4 and resid 317 and name CA)	7.06	0.70	0.70
	assign (segid 3A4 and resid 313 and name CG)	(segid 3A4 and resid 317 and name N)	7.05	0.42	0.43
55	assign (segid 3A4 and resid 313 and name CG)	(segid 3A4 and resid 383 and name C)	6.76	0.27	0.26
	assign (segid 3A4 and resid 313 and name CG)	(segid 3A4 and resid 383 and name CA)	6.43	0.27	0.27
	assign (segid 3A4 and resid 313 and name CG)	(segid 3A4 and resid 383 and name N)	7.17	0.23	0.24
	assign (segid 3A4 and resid 313 and name CG)	(segid 3A4 and resid 383 and name O)	6.98	0.34	0.34
	assign (segid 3A4 and resid 313 and name CG)	(segid 3A4 and resid 384 and name CD1)	6.01	0.49	0.49
60	assign (segid 3A4 and resid 313 and name CG)	(segid 3A4 and resid 384 and name CD2)	6.20	0.55	0.54
	assign (segid 3A4 and resid 313 and name CG)	(segid 3A4 and resid 384 and name CG)	6.51	0.35	0.36
	assign (segid 3A4 and resid 313 and name CG)	(segid 3A4 and resid 384 and name N)	7.16	0.21	0.20
	assign (segid 3A4 and resid 313 and name CG)	(segid 3A4 and resid 398 and name CG)	6.28	0.67	0.66
	assign (segid 3A4 and resid 313 and name CG)	(segid HEM and resid 1 and name C2B)	6.75	0.39	0.38
65	assign (segid 3A4 and resid 313 and name CG)	(segid HEM and resid 1 and name C3B)	6.91	0.40	0.40
	assign (segid 3A4 and resid 313 and name CG)	(segid HEM and resid 1 and name CAB)	6.31	0.40	0.39
	assign (segid 3A4 and resid 313 and name CG)	(segid HEM and resid 1 and name CBB)	5.25	0.54	0.53
	assign (segid 3A4 and resid 313 and name CG)	(segid HEM and resid 1 and name CMB)	5.80	0.43	0.43
	assign (segid 3A4 and resid 313 and name CG)	(segid 3A4 and resid 313 and name C)	2.45	0.04	0.03
70	assign (segid 3A4 and resid 313 and name N)	(segid 3A4 and resid 313 and name CA)	1.47	0.02	0.01
	assign (segid 3A4 and resid 313 and name N)	(segid 3A4 and resid 313 and name CB)	2.45	0.01	0.02
	assign (segid 3A4 and resid 313 and name N)	(segid 3A4 and resid 313 and name CG)	3.12	0.13	0.13
	assign (segid 3A4 and resid 313 and name N)	(segid 3A4 and resid 313 and name O)	3.53	0.04	0.04
	assign (segid 3A4 and resid 313 and name N)	(segid 3A4 and resid 314 and name C)	4.71	0.05	0.04
75	assign (segid 3A4 and resid 313 and name N)	(segid 3A4 and resid 314 and name CA)	4.20	0.06	0.06
	assign (segid 3A4 and resid 313 and name N)	(segid 3A4 and resid 314 and name CB)	4.98	0.09	0.09
	assign (segid 3A4 and resid 313 and name N)	(segid 3A4 and resid 314 and name CG)	6.45	0.09	0.10
	assign (segid 3A4 and resid 313 and name N)	(segid 3A4 and resid 314 and name N)	2.78	0.05	0.06
	assign (segid 3A4 and resid 313 and name N)	(segid 3A4 and resid 314 and name O)	5.68	0.06	0.06
80	assign (segid 3A4 and resid 313 and name N)	(segid 3A4 and resid 315 and name C)	5.68	0.05	0.06
	assign (segid 3A4 and resid 313 and name N)	(segid 3A4 and resid 315 and name CA)	5.45	0.05	0.05
	assign (segid 3A4 and resid 313 and name N)	(segid 3A4 and resid 315 and name CB)	5.66	0.11	0.11

	assign (segid 3A4 and resid 313 and name N)	(segid 3A4 and resid 315 and name N)	4.44	0.06	0.06
	assign (segid 3A4 and resid 313 and name N)	(segid 3A4 and resid 315 and name O)	6.87	0.05	0.06
	assign (segid 3A4 and resid 313 and name N)	(segid 3A4 and resid 316 and name C)	5.70	0.35	0.34
	assign (segid 3A4 and resid 313 and name N)	(segid 3A4 and resid 316 and name CA)	5.66	0.15	0.14
5	assign (segid 3A4 and resid 313 and name N)	(segid 3A4 and resid 316 and name N)	4.88	0.11	0.10
	assign (segid 3A4 and resid 313 and name N)	(segid 3A4 and resid 316 and name O)	5.96	0.92	0.92
	assign (segid 3A4 and resid 313 and name N)	(segid 3A4 and resid 317 and name C)	7.45	0.35	0.35
	assign (segid 3A4 and resid 313 and name N)	(segid 3A4 and resid 317 and name CA)	6.44	0.39	0.39
	assign (segid 3A4 and resid 313 and name N)	(segid 3A4 and resid 317 and name N)	5.86	0.24	0.23
10	assign (segid 3A4 and resid 313 and name N)	(segid 3A4 and resid 383 and name CA)	7.54	0.29	0.29
	assign (segid 3A4 and resid 313 and name O)	(segid 3A4 and resid 313 and name CB)	3.19	0.07	0.07
	assign (segid 3A4 and resid 313 and name O)	(segid 3A4 and resid 313 and name CG)	4.53	0.06	0.06
	assign (segid 3A4 and resid 313 and name O)	(segid 3A4 and resid 314 and name C)	3.09	0.15	0.15
	assign (segid 3A4 and resid 313 and name O)	(segid 3A4 and resid 314 and name CA)	2.75	0.06	0.05
15	assign (segid 3A4 and resid 313 and name O)	(segid 3A4 and resid 314 and name CB)	4.22	0.06	0.06
	assign (segid 3A4 and resid 313 and name O)	(segid 3A4 and resid 314 and name CG)	5.21	0.07	0.07
	assign (segid 3A4 and resid 313 and name O)	(segid 3A4 and resid 314 and name N)	2.24	0.03	0.03
	assign (segid 3A4 and resid 313 and name O)	(segid 3A4 and resid 314 and name O)	3.40	0.17	0.16
20	assign (segid 3A4 and resid 313 and name O)	(segid 3A4 and resid 315 and name C)	4.66	0.28	0.27
	assign (segid 3A4 and resid 313 and name O)	(segid 3A4 and resid 315 and name CA)	4.80	0.25	0.25
	assign (segid 3A4 and resid 313 and name O)	(segid 3A4 and resid 315 and name CB)	5.89	0.25	0.25
	assign (segid 3A4 and resid 313 and name O)	(segid 3A4 and resid 315 and name N)	3.78	0.21	0.21
	assign (segid 3A4 and resid 313 and name O)	(segid 3A4 and resid 315 and name O)	5.51	0.30	0.30
25	assign (segid 3A4 and resid 313 and name O)	(segid 3A4 and resid 316 and name C)	4.03	0.19	0.20
	assign (segid 3A4 and resid 313 and name O)	(segid 3A4 and resid 316 and name CA)	4.61	0.23	0.23
	assign (segid 3A4 and resid 313 and name O)	(segid 3A4 and resid 316 and name N)	4.08	0.26	0.26
	assign (segid 3A4 and resid 313 and name O)	(segid 3A4 and resid 316 and name O)	4.57	0.50	0.49
	assign (segid 3A4 and resid 313 and name O)	(segid 3A4 and resid 317 and name C)	4.98	0.25	0.25
30	assign (segid 3A4 and resid 313 and name O)	(segid 3A4 and resid 317 and name CA)	3.68	0.31	0.30
	assign (segid 3A4 and resid 313 and name O)	(segid 3A4 and resid 317 and name N)	3.48	0.39	0.38
	assign (segid 3A4 and resid 313 and name O)	(segid 3A4 and resid 317 and name O)	5.99	0.28	0.29
	assign (segid 3A4 and resid 313 and name O)	(segid 3A4 and resid 318 and name CA)	6.64	0.33	0.33
	assign (segid 3A4 and resid 313 and name O)	(segid 3A4 and resid 318 and name CB)	6.93	0.47	0.46
35	assign (segid 3A4 and resid 313 and name O)	(segid 3A4 and resid 318 and name N)	5.27	0.31	0.31
	assign (segid 3A4 and resid 313 and name O)	(segid 3A4 and resid 319 and name N)	7.39	0.25	0.25
	assign (segid 3A4 and resid 313 and name O)	(segid 3A4 and resid 351 and name CA)	6.98	0.18	0.18
	assign (segid 3A4 and resid 313 and name O)	(segid 3A4 and resid 351 and name O)	7.55	0.27	0.26
	assign (segid 3A4 and resid 313 and name O)	(segid 3A4 and resid 381 and name CA)	7.12	0.44	0.45
40	assign (segid 3A4 and resid 313 and name O)	(segid 3A4 and resid 382 and name C)	6.59	0.46	0.46
	assign (segid 3A4 and resid 313 and name O)	(segid 3A4 and resid 382 and name N)	6.92	0.43	0.44
	assign (segid 3A4 and resid 313 and name O)	(segid 3A4 and resid 382 and name O)	7.14	0.43	0.43
	assign (segid 3A4 and resid 313 and name O)	(segid 3A4 and resid 383 and name C)	6.02	0.54	0.55
	assign (segid 3A4 and resid 313 and name O)	(segid 3A4 and resid 383 and name CA)	4.88	0.53	0.53
45	assign (segid 3A4 and resid 313 and name O)	(segid 3A4 and resid 383 and name N)	5.48	0.51	0.50
	assign (segid 3A4 and resid 313 and name O)	(segid 3A4 and resid 383 and name O)	6.33	0.51	0.50
	assign (segid 3A4 and resid 313 and name O)	(segid 3A4 and resid 384 and name N)	6.94	0.58	0.58
	assign (segid 3A4 and resid 313 and name O)	(segid HEM and resid 1 and name CMB)	6.74	0.47	0.47
	assign (segid 3A4 and resid 314 and name C)	(segid 3A4 and resid 314 and name CB)	2.48	0.02	0.01
	assign (segid 3A4 and resid 314 and name C)	(segid 3A4 and resid 314 and name CG)	3.00	0.03	0.04
50	assign (segid 3A4 and resid 314 and name C)	(segid 3A4 and resid 314 and name O)	1.24	0.01	0.00
	assign (segid 3A4 and resid 314 and name C)	(segid 3A4 and resid 315 and name C)	3.10	0.06	0.05
	assign (segid 3A4 and resid 314 and name C)	(segid 3A4 and resid 315 and name CA)	2.44	0.01	0.01
	assign (segid 3A4 and resid 314 and name C)	(segid 3A4 and resid 315 and name CB)	3.71	0.02	0.02
	assign (segid 3A4 and resid 314 and name C)	(segid 3A4 and resid 315 and name N)	1.34	0.01	0.01
55	assign (segid 3A4 and resid 314 and name C)	(segid 3A4 and resid 315 and name O)	3.90	0.13	0.12
	assign (segid 3A4 and resid 314 and name C)	(segid 3A4 and resid 316 and name C)	4.82	0.14	0.14
	assign (segid 3A4 and resid 314 and name C)	(segid 3A4 and resid 316 and name CA)	4.67	0.08	0.07
	assign (segid 3A4 and resid 314 and name C)	(segid 3A4 and resid 316 and name N)	3.48	0.05	0.05
	assign (segid 3A4 and resid 314 and name C)	(segid 3A4 and resid 316 and name O)	5.69	0.33	0.33
60	assign (segid 3A4 and resid 314 and name C)	(segid 3A4 and resid 317 and name C)	6.58	0.30	0.29
	assign (segid 3A4 and resid 314 and name C)	(segid 3A4 and resid 317 and name CA)	5.15	0.28	0.28
	assign (segid 3A4 and resid 314 and name C)	(segid 3A4 and resid 317 and name N)	4.39	0.29	0.30
	assign (segid 3A4 and resid 314 and name C)	(segid 3A4 and resid 317 and name O)	7.25	0.32	0.33
	assign (segid 3A4 and resid 314 and name C)	(segid 3A4 and resid 318 and name N)	7.28	0.36	0.36
65	assign (segid 3A4 and resid 314 and name C)	(segid 3A4 and resid 347 and name O)	7.19	0.43	0.43
	assign (segid 3A4 and resid 314 and name C)	(segid 3A4 and resid 348 and name CA)	7.09	0.44	0.44
	assign (segid 3A4 and resid 314 and name C)	(segid 3A4 and resid 348 and name O)	6.58	0.46	0.47
	assign (segid 3A4 and resid 314 and name C)	(segid 3A4 and resid 351 and name C)	5.52	0.17	0.18
	assign (segid 3A4 and resid 314 and name C)	(segid 3A4 and resid 351 and name CA)	5.44	0.13	0.13
70	assign (segid 3A4 and resid 314 and name C)	(segid 3A4 and resid 351 and name N)	6.55	0.21	0.21
	assign (segid 3A4 and resid 314 and name C)	(segid 3A4 and resid 351 and name O)	5.11	0.18	0.18
	assign (segid 3A4 and resid 314 and name C)	(segid 3A4 and resid 352 and name CA)	7.05	0.34	0.33
	assign (segid 3A4 and resid 314 and name C)	(segid 3A4 and resid 352 and name CB)	7.26	0.32	0.33
	assign (segid 3A4 and resid 314 and name C)	(segid 3A4 and resid 352 and name CG)	6.22	0.32	0.32
75	assign (segid 3A4 and resid 314 and name C)	(segid 3A4 and resid 352 and name N)	6.43	0.30	0.30
	assign (segid 3A4 and resid 314 and name C)	(segid 3A4 and resid 360 and name O)	6.60	0.18	0.19
	assign (segid 3A4 and resid 314 and name C)	(segid 3A4 and resid 383 and name CA)	7.12	0.45	0.44
	assign (segid 3A4 and resid 314 and name CA)	(segid 3A4 and resid 314 and name C)	1.52	0.01	0.01
80	assign (segid 3A4 and resid 314 and name CA)	(segid 3A4 and resid 314 and name CB)	1.53	0.00	0.00
	assign (segid 3A4 and resid 314 and name CA)	(segid 3A4 and resid 314 and name O)	2.56	0.01	0.02
	assign (segid 3A4 and resid 314 and name CA)	(segid 3A4 and resid 314 and name O)	2.41	0.02	0.02
	assign (segid 3A4 and resid 314 and name CA)	(segid 3A4 and resid 315 and name C)	4.50	0.06	0.06
	assign (segid 3A4 and resid 314 and name CA)	(segid 3A4 and resid 315 and name CA)	3.79	0.01	0.02

	assign	(segid 3A4 and resid 314 and name CA)	(segid 3A4 and resid 315 and name CB)	4.81	0.04	0.05
	assign	(segid 3A4 and resid 314 and name CA)	(segid 3A4 and resid 315 and name N)	2.42	0.02	0.01
	assign	(segid 3A4 and resid 314 and name CA)	(segid 3A4 and resid 315 and name O)	5.38	0.13	0.12
	assign	(segid 3A4 and resid 314 and name CA)	(segid 3A4 and resid 316 and name C)	5.69	0.16	0.16
5	assign	(segid 3A4 and resid 314 and name CA)	(segid 3A4 and resid 316 and name CA)	5.74	0.09	0.09
	assign	(segid 3A4 and resid 314 and name CA)	(segid 3A4 and resid 316 and name N)	4.62	0.07	0.06
	assign	(segid 3A4 and resid 314 and name CA)	(segid 3A4 and resid 316 and name O)	6.44	0.46	0.46
	assign	(segid 3A4 and resid 314 and name CA)	(segid 3A4 and resid 317 and name C)	7.12	0.21	0.22
	assign	(segid 3A4 and resid 314 and name CA)	(segid 3A4 and resid 317 and name CA)	5.67	0.19	0.19
10	assign	(segid 3A4 and resid 314 and name CA)	(segid 3A4 and resid 317 and name N)	5.18	0.26	0.25
	assign	(segid 3A4 and resid 314 and name CA)	(segid 3A4 and resid 318 and name CA)	9.06	0.29	0.30
	assign	(segid 3A4 and resid 314 and name CA)	(segid 3A4 and resid 318 and name CB)	9.46	0.42	0.41
	assign	(segid 3A4 and resid 314 and name CA)	(segid 3A4 and resid 319 and name CA)	10.85	0.33	0.33
	assign	(segid 3A4 and resid 314 and name CA)	(segid 3A4 and resid 319 and name CB)	11.13	0.37	0.38
15	assign	(segid 3A4 and resid 314 and name CA)	(segid 3A4 and resid 322 and name CA)	19.10	0.36	0.36
	assign	(segid 3A4 and resid 314 and name CA)	(segid 3A4 and resid 344 and name CA)	18.23	0.27	0.27
	assign	(segid 3A4 and resid 314 and name CA)	(segid 3A4 and resid 344 and name CB)	18.39	0.20	0.20
	assign	(segid 3A4 and resid 314 and name CA)	(segid 3A4 and resid 345 and name CA)	15.08	0.44	0.44
	assign	(segid 3A4 and resid 314 and name CA)	(segid 3A4 and resid 345 and name CB)	14.95	0.66	0.67
20	assign	(segid 3A4 and resid 314 and name CA)	(segid 3A4 and resid 346 and name CA)	12.50	0.27	0.26
	assign	(segid 3A4 and resid 314 and name CA)	(segid 3A4 and resid 346 and name CB)	12.94	0.25	0.25
	assign	(segid 3A4 and resid 314 and name CA)	(segid 3A4 and resid 347 and name CA)	9.20	0.37	0.37
	assign	(segid 3A4 and resid 314 and name CA)	(segid 3A4 and resid 347 and name CB)	8.97	0.44	0.44
	assign	(segid 3A4 and resid 314 and name CA)	(segid 3A4 and resid 347 and name O)	7.37	0.31	0.31
25	assign	(segid 3A4 and resid 314 and name CA)	(segid 3A4 and resid 348 and name CA)	7.76	0.32	0.32
	assign	(segid 3A4 and resid 314 and name CA)	(segid 3A4 and resid 349 and name CA)	9.89	0.41	0.42
	assign	(segid 3A4 and resid 314 and name CA)	(segid 3A4 and resid 349 and name CB)	11.35	0.39	0.38
	assign	(segid 3A4 and resid 314 and name CA)	(segid 3A4 and resid 350 and name CA)	9.05	0.22	0.22
	assign	(segid 3A4 and resid 314 and name CA)	(segid 3A4 and resid 350 and name CB)	9.18	0.29	0.29
30	assign	(segid 3A4 and resid 314 and name CA)	(segid 3A4 and resid 351 and name C)	5.92	0.22	0.22
	assign	(segid 3A4 and resid 314 and name CA)	(segid 3A4 and resid 351 and name CA)	5.55	0.15	0.16
	assign	(segid 3A4 and resid 314 and name CA)	(segid 3A4 and resid 351 and name N)	6.70	0.20	0.20
	assign	(segid 3A4 and resid 314 and name CA)	(segid 3A4 and resid 351 and name O)	5.49	0.23	0.24
	assign	(segid 3A4 and resid 314 and name CA)	(segid 3A4 and resid 352 and name CA)	7.78	0.33	0.33
35	assign	(segid 3A4 and resid 314 and name CA)	(segid 3A4 and resid 352 and name CB)	8.23	0.33	0.33
	assign	(segid 3A4 and resid 314 and name CA)	(segid 3A4 and resid 352 and name CG)	7.34	0.33	0.33
	assign	(segid 3A4 and resid 314 and name CA)	(segid 3A4 and resid 352 and name N)	7.00	0.31	0.32
	assign	(segid 3A4 and resid 314 and name CA)	(segid 3A4 and resid 353 and name CA)	10.66	0.31	0.31
	assign	(segid 3A4 and resid 314 and name CA)	(segid 3A4 and resid 353 and name CB)	10.96	0.30	0.30
40	assign	(segid 3A4 and resid 314 and name CA)	(segid 3A4 and resid 354 and name CA)	12.71	0.38	0.37
	assign	(segid 3A4 and resid 314 and name CA)	(segid 3A4 and resid 354 and name CB)	13.88	0.43	0.42
	assign	(segid 3A4 and resid 314 and name CA)	(segid 3A4 and resid 355 and name CA)	14.44	0.32	0.31
	assign	(segid 3A4 and resid 314 and name CA)	(segid 3A4 and resid 355 and name CB)	15.21	0.29	0.30
	assign	(segid 3A4 and resid 314 and name CA)	(segid 3A4 and resid 356 and name CA)	11.64	0.38	0.38
45	assign	(segid 3A4 and resid 314 and name CA)	(segid 3A4 and resid 356 and name CB)	10.78	0.41	0.41
	assign	(segid 3A4 and resid 314 and name CA)	(segid 3A4 and resid 357 and name CA)	9.79	0.32	0.31
	assign	(segid 3A4 and resid 314 and name CA)	(segid 3A4 and resid 357 and name CB)	8.35	0.37	0.36
	assign	(segid 3A4 and resid 314 and name CA)	(segid 3A4 and resid 358 and name CA)	12.78	0.51	0.51
	assign	(segid 3A4 and resid 314 and name CA)	(segid 3A4 and resid 358 and name CB)	13.82	0.69	0.70
50	assign	(segid 3A4 and resid 314 and name CA)	(segid 3A4 and resid 359 and name CA)	12.35	0.15	0.16
	assign	(segid 3A4 and resid 314 and name CA)	(segid 3A4 and resid 359 and name CB)	12.98	0.13	0.13
	assign	(segid 3A4 and resid 314 and name CA)	(segid 3A4 and resid 360 and name CA)	9.01	0.16	0.17
	assign	(segid 3A4 and resid 314 and name CA)	(segid 3A4 and resid 360 and name CB)	9.21	0.23	0.24
	assign	(segid 3A4 and resid 314 and name CA)	(segid 3A4 and resid 360 and name O)	7.59	0.17	0.16
55	assign	(segid 3A4 and resid 314 and name CA)	(segid 3A4 and resid 361 and name CA)	9.94	0.18	0.17
	assign	(segid 3A4 and resid 314 and name CA)	(segid 3A4 and resid 361 and name CB)	11.22	0.20	0.20
	assign	(segid 3A4 and resid 314 and name CA)	(segid 3A4 and resid 362 and name CA)	10.54	0.13	0.13
	assign	(segid 3A4 and resid 314 and name CA)	(segid 3A4 and resid 362 and name CB)	11.56	0.11	0.10
	assign	(segid 3A4 and resid 314 and name CA)	(segid 3A4 and resid 363 and name CA)	8.99	0.09	0.09
60	assign	(segid 3A4 and resid 314 and name CA)	(segid 3A4 and resid 363 and name CB)	9.33	0.15	0.16
	assign	(segid 3A4 and resid 314 and name CA)	(segid 3A4 and resid 364 and name CA)	10.23	0.11	0.11
	assign	(segid 3A4 and resid 314 and name CA)	(segid 3A4 and resid 364 and name CB)	10.83	0.12	0.13
	assign	(segid 3A4 and resid 314 and name CA)	(segid 3A4 and resid 365 and name CA)	10.28	0.26	0.25
	assign	(segid 3A4 and resid 314 and name CA)	(segid 3A4 and resid 365 and name CB)	11.16	0.22	0.22
65	assign	(segid 3A4 and resid 314 and name CA)	(segid 3A4 and resid 381 and name C)	6.73	0.45	0.44
	assign	(segid 3A4 and resid 314 and name CA)	(segid 3A4 and resid 381 and name CA)	6.03	0.49	0.48
	assign	(segid 3A4 and resid 314 and name CA)	(segid 3A4 and resid 382 and name CA)	7.66	0.40	0.40
	assign	(segid 3A4 and resid 314 and name CA)	(segid 3A4 and resid 382 and name CB)	8.66	0.45	0.45
	assign	(segid 3A4 and resid 314 and name CA)	(segid 3A4 and resid 382 and name N)	6.66	0.39	0.38
70	assign	(segid 3A4 and resid 314 and name CA)	(segid 3A4 and resid 383 and name CA)	6.34	0.46	0.46
	assign	(segid 3A4 and resid 314 and name CA)	(segid 3A4 and resid 383 and name N)	6.33	0.46	0.45
	assign	(segid 3A4 and resid 314 and name CA)	(segid 3A4 and resid 384 and name CA)	9.77	0.52	0.52
	assign	(segid 3A4 and resid 314 and name CA)	(segid 3A4 and resid 384 and name CB)	10.19	0.55	0.55
	assign	(segid 3A4 and resid 314 and name CA)	(segid 3A4 and resid 385 and name CA)	11.58	0.51	0.50
75	assign	(segid 3A4 and resid 314 and name CA)	(segid 3A4 and resid 386 and name CA)	13.84	0.56	0.56
	assign	(segid 3A4 and resid 314 and name CA)	(segid 3A4 and resid 387 and name CA)	17.45	0.42	0.41
	assign	(segid 3A4 and resid 314 and name CA)	(segid 3A4 and resid 389 and name CA)	18.48	0.55	0.55
	assign	(segid 3A4 and resid 314 and name CA)	(segid 3A4 and resid 389 and name CB)	18.62	0.61	0.61
	assign	(segid 3A4 and resid 314 and name CA)	(segid 3A4 and resid 390 and name CA)	15.34	0.46	0.46
80	assign	(segid 3A4 and resid 314 and name CA)	(segid 3A4 and resid 390 and name CB)	15.23	0.42	0.41
	assign	(segid 3A4 and resid 314 and name CA)	(segid 3A4 and resid 391 and name CA)	14.79	0.49	0.50
	assign	(segid 3A4 and resid 314 and name CA)	(segid 3A4 and resid 391 and name CB)	13.54	0.50	0.50
	assign	(segid 3A4 and resid 314 and name CA)	(segid 3A4 and resid 392 and name CA)	17.86	0.51	0.50

	assign (segid 3A4 and resid 314 and name CA) (segid 3A4 and resid 393 and name CA)	16.72	0.52	0.53
	assign (segid 3A4 and resid 314 and name CA) (segid 3A4 and resid 394 and name CA)	13.65	0.55	0.54
	assign (segid 3A4 and resid 314 and name CA) (segid 3A4 and resid 394 and name CB)	13.24	0.65	0.65
	assign (segid 3A4 and resid 314 and name CA) (segid 3A4 and resid 395 and name CA)	15.88	0.60	0.60
	assign (segid 3A4 and resid 314 and name CA) (segid 3A4 and resid 396 and name CA)	17.24	0.54	0.55
5	assign (segid 3A4 and resid 314 and name CA) (segid 3A4 and resid 396 and name CB)	18.16	0.57	0.56
	assign (segid 3A4 and resid 314 and name CA) (segid 3A4 and resid 397 and name CA)	14.02	0.56	0.56
	assign (segid 3A4 and resid 314 and name CA) (segid 3A4 and resid 397 and name CB)	13.03	0.58	0.58
	assign (segid 3A4 and resid 314 and name CA) (segid 3A4 and resid 398 and name CA)	12.82	0.52	0.51
	assign (segid 3A4 and resid 314 and name CA) (segid 3A4 and resid 398 and name CB)	12.58	0.53	0.53
10	assign (segid 3A4 and resid 314 and name CA) (segid 3A4 and resid 399 and name CA)	16.39	0.49	0.50
	assign (segid 3A4 and resid 314 and name CA) (segid 3A4 and resid 399 and name CB)	17.62	0.50	0.49
	assign (segid 3A4 and resid 314 and name CA) (segid 3A4 and resid 400 and name CA)	16.74	0.50	0.51
	assign (segid 3A4 and resid 314 and name CA) (segid 3A4 and resid 400 and name CB)	16.77	0.48	0.48
	assign (segid 3A4 and resid 314 and name CA) (segid 3A4 and resid 401 and name CA)	13.75	0.52	0.52
15	assign (segid 3A4 and resid 314 and name CA) (segid 3A4 and resid 402 and name CA)	15.00	0.42	0.41
	assign (segid 3A4 and resid 314 and name CA) (segid 3A4 and resid 402 and name CB)	15.15	0.40	0.40
	assign (segid 3A4 and resid 314 and name CA) (segid 3A4 and resid 403 and name CA)	18.55	0.44	0.44
	assign (segid 3A4 and resid 314 and name CA) (segid 3A4 and resid 404 and name CA)	18.14	0.57	0.56
	assign (segid 3A4 and resid 314 and name CA) (segid 3A4 and resid 404 and name CB)	17.41	0.69	0.68
20	assign (segid 3A4 and resid 314 and name CA) (segid 3A4 and resid 405 and name CA)	16.40	0.36	0.35
	assign (segid 3A4 and resid 314 and name CA) (segid 3A4 and resid 405 and name CB)	14.99	0.36	0.36
	assign (segid 3A4 and resid 314 and name CA) (segid 3A4 and resid 406 and name CA)	18.85	0.38	0.38
	assign (segid 3A4 and resid 314 and name CA) (segid 3A4 and resid 427 and name CA)	17.00	0.84	0.84
	assign (segid 3A4 and resid 314 and name CA) (segid 3A4 and resid 429 and name CA)	17.70	0.52	0.53
25	assign (segid 3A4 and resid 314 and name CA) (segid 3A4 and resid 430 and name CA)	17.80	1.12	1.12
	assign (segid 3A4 and resid 314 and name CA) (segid 3A4 and resid 431 and name CA)	16.55	0.73	0.72
	assign (segid 3A4 and resid 314 and name CA) (segid 3A4 and resid 433 and name CA)	13.03	0.51	0.50
	assign (segid 3A4 and resid 314 and name CA) (segid 3A4 and resid 434 and name CA)	13.85	0.95	0.94
	assign (segid 3A4 and resid 314 and name CA) (segid 3A4 and resid 435 and name CA)	15.59	1.00	1.00
30	assign (segid 3A4 and resid 314 and name CA) (segid 3A4 and resid 314 and name CG)	1.52	0.01	0.01
	assign (segid 3A4 and resid 314 and name CB) (segid 3A4 and resid 315 and name C)	5.39	0.06	0.07
	assign (segid 3A4 and resid 314 and name CB) (segid 3A4 and resid 315 and name CA)	4.33	0.05	0.04
	assign (segid 3A4 and resid 314 and name CB) (segid 3A4 and resid 315 and name CB)	5.08	0.08	0.07
	assign (segid 3A4 and resid 314 and name CB) (segid 3A4 and resid 315 and name N)	3.01	0.04	0.04
35	assign (segid 3A4 and resid 314 and name CB) (segid 3A4 and resid 315 and name O)	6.24	0.12	0.12
	assign (segid 3A4 and resid 314 and name CB) (segid 3A4 and resid 316 and name C)	7.09	0.14	0.15
	assign (segid 3A4 and resid 314 and name CB) (segid 3A4 and resid 316 and name CA)	6.99	0.09	0.09
	assign (segid 3A4 and resid 314 and name CB) (segid 3A4 and resid 316 and name N)	5.72	0.07	0.08
	assign (segid 3A4 and resid 314 and name CB) (segid 3A4 and resid 317 and name CA)	7.14	0.22	0.22
40	assign (segid 3A4 and resid 314 and name CB) (segid 3A4 and resid 317 and name N)	6.63	0.27	0.27
	assign (segid 3A4 and resid 314 and name CB) (segid 3A4 and resid 318 and name CA)	10.57	0.29	0.29
	assign (segid 3A4 and resid 314 and name CB) (segid 3A4 and resid 318 and name CB)	10.95	0.40	0.40
	assign (segid 3A4 and resid 314 and name CB) (segid 3A4 and resid 319 and name CA)	12.29	0.34	0.35
	assign (segid 3A4 and resid 314 and name CB) (segid 3A4 and resid 319 and name CB)	12.54	0.40	0.40
45	assign (segid 3A4 and resid 314 and name CB) (segid 3A4 and resid 344 and name CA)	19.15	0.22	0.21
	assign (segid 3A4 and resid 314 and name CB) (segid 3A4 and resid 344 and name CB)	19.36	0.16	0.15
	assign (segid 3A4 and resid 314 and name CB) (segid 3A4 and resid 345 and name CA)	15.88	0.37	0.37
	assign (segid 3A4 and resid 314 and name CB) (segid 3A4 and resid 345 and name CB)	15.71	0.60	0.61
	assign (segid 3A4 and resid 314 and name CB) (segid 3A4 and resid 346 and name CA)	13.35	0.20	0.21
50	assign (segid 3A4 and resid 314 and name CB) (segid 3A4 and resid 346 and name CB)	13.75	0.18	0.18
	assign (segid 3A4 and resid 314 and name CB) (segid 3A4 and resid 347 and name CA)	10.07	0.33	0.33
	assign (segid 3A4 and resid 314 and name CB) (segid 3A4 and resid 347 and name CB)	9.96	0.41	0.42
	assign (segid 3A4 and resid 314 and name CB) (segid 3A4 and resid 348 and name CA)	8.70	0.26	0.26
	assign (segid 3A4 and resid 314 and name CB) (segid 3A4 and resid 349 and name CA)	10.36	0.35	0.36
55	assign (segid 3A4 and resid 314 and name CB) (segid 3A4 and resid 349 and name CB)	11.83	0.34	0.33
	assign (segid 3A4 and resid 314 and name CB) (segid 3A4 and resid 350 and name CA)	9.19	0.25	0.25
	assign (segid 3A4 and resid 314 and name CB) (segid 3A4 and resid 350 and name CB)	9.39	0.32	0.33
	assign (segid 3A4 and resid 314 and name CB) (segid 3A4 and resid 351 and name C)	5.73	0.24	0.23
	assign (segid 3A4 and resid 314 and name CB) (segid 3A4 and resid 351 and name CA)	5.53	0.20	0.21
60	assign (segid 3A4 and resid 314 and name CB) (segid 3A4 and resid 351 and name N)	6.84	0.25	0.25
	assign (segid 3A4 and resid 314 and name CB) (segid 3A4 and resid 351 and name O)	5.05	0.23	0.24
	assign (segid 3A4 and resid 314 and name CB) (segid 3A4 and resid 352 and name CA)	7.58	0.32	0.32
	assign (segid 3A4 and resid 314 and name CB) (segid 3A4 and resid 352 and name CB)	8.24	0.30	0.31
	assign (segid 3A4 and resid 314 and name CB) (segid 3A4 and resid 352 and name N)	6.91	0.31	0.31
65	assign (segid 3A4 and resid 314 and name CB) (segid 3A4 and resid 353 and name CA)	10.21	0.33	0.33
	assign (segid 3A4 and resid 314 and name CB) (segid 3A4 and resid 353 and name CB)	10.52	0.35	0.35
	assign (segid 3A4 and resid 314 and name CB) (segid 3A4 and resid 354 and name CA)	11.92	0.38	0.38
	assign (segid 3A4 and resid 314 and name CB) (segid 3A4 and resid 354 and name CB)	13.13	0.43	0.44
	assign (segid 3A4 and resid 314 and name CB) (segid 3A4 and resid 355 and name CA)	13.54	0.36	0.36
70	assign (segid 3A4 and resid 314 and name CB) (segid 3A4 and resid 355 and name CB)	14.40	0.33	0.34
	assign (segid 3A4 and resid 314 and name CB) (segid 3A4 and resid 356 and name CA)	10.62	0.41	0.41
	assign (segid 3A4 and resid 314 and name CB) (segid 3A4 and resid 356 and name CB)	9.88	0.44	0.43
	assign (segid 3A4 and resid 314 and name CB) (segid 3A4 and resid 357 and name CA)	8.58	0.31	0.32
	assign (segid 3A4 and resid 314 and name CB) (segid 3A4 and resid 357 and name CB)	7.18	0.37	0.37
75	assign (segid 3A4 and resid 314 and name CB) (segid 3A4 and resid 358 and name CA)	11.59	0.54	0.54
	assign (segid 3A4 and resid 314 and name CB) (segid 3A4 and resid 358 and name CB)	12.57	0.75	0.75
	assign (segid 3A4 and resid 314 and name CB) (segid 3A4 and resid 359 and name CA)	11.36	0.16	0.17
	assign (segid 3A4 and resid 314 and name CB) (segid 3A4 and resid 359 and name CB)	11.94	0.19	0.19
80	assign (segid 3A4 and resid 314 and name CB) (segid 3A4 and resid 360 and name CA)	8.23	0.14	0.15
	assign (segid 3A4 and resid 314 and name CB) (segid 3A4 and resid 360 and name CB)	8.54	0.21	0.20
	assign (segid 3A4 and resid 314 and name CB) (segid 3A4 and resid 360 and name O)	7.05	0.20	0.20
	assign (segid 3A4 and resid 314 and name CB) (segid 3A4 and resid 361 and name CA)	9.56	0.23	0.24

	assign (segid 3A4 and resid 314 and name CB)	(segid 3A4 and resid 361 and name CB)	10.93	0.25	0.25
	assign (segid 3A4 and resid 314 and name CB)	(segid 3A4 and resid 362 and name CA)	9.88	0.16	0.17
	assign (segid 3A4 and resid 314 and name CB)	(segid 3A4 and resid 362 and name CB)	10.75	0.12	0.12
	assign (segid 3A4 and resid 314 and name CB)	(segid 3A4 and resid 362 and name O)	7.78	0.16	0.16
5	assign (segid 3A4 and resid 314 and name CB)	(segid 3A4 and resid 363 and name CA)	8.41	0.06	0.07
	assign (segid 3A4 and resid 314 and name CB)	(segid 3A4 and resid 363 and name CB)	8.97	0.10	0.10
	assign (segid 3A4 and resid 314 and name CB)	(segid 3A4 and resid 364 and name CA)	9.22	0.13	0.14
	assign (segid 3A4 and resid 314 and name CB)	(segid 3A4 and resid 364 and name CB)	9.71	0.16	0.17
	assign (segid 3A4 and resid 314 and name CB)	(segid 3A4 and resid 364 and name O)	9.31	0.31	0.31
	assign (segid 3A4 and resid 314 and name CB)	(segid 3A4 and resid 365 and name CA)	10.33	0.29	0.28
10	assign (segid 3A4 and resid 314 and name CB)	(segid 3A4 and resid 365 and name CB)	6.72	0.53	0.53
	assign (segid 3A4 and resid 314 and name CB)	(segid 3A4 and resid 381 and name C)	5.73	0.57	0.57
	assign (segid 3A4 and resid 314 and name CB)	(segid 3A4 and resid 382 and name CA)	8.08	0.47	0.47
	assign (segid 3A4 and resid 314 and name CB)	(segid 3A4 and resid 382 and name CB)	9.06	0.51	0.52
15	assign (segid 3A4 and resid 314 and name CB)	(segid 3A4 and resid 382 and name N)	6.89	0.47	0.47
	assign (segid 3A4 and resid 314 and name CB)	(segid 3A4 and resid 383 and name CA)	7.35	0.49	0.49
	assign (segid 3A4 and resid 314 and name CB)	(segid 3A4 and resid 384 and name CA)	10.65	0.58	0.57
	assign (segid 3A4 and resid 314 and name CB)	(segid 3A4 and resid 384 and name CB)	10.96	0.62	0.61
	assign (segid 3A4 and resid 314 and name CB)	(segid 3A4 and resid 385 and name CA)	12.34	0.59	0.59
	assign (segid 3A4 and resid 314 and name CB)	(segid 3A4 and resid 386 and name CA)	14.27	0.69	0.68
20	assign (segid 3A4 and resid 314 and name CB)	(segid 3A4 and resid 387 and name CA)	17.83	0.51	0.52
	assign (segid 3A4 and resid 314 and name CB)	(segid 3A4 and resid 390 and name CA)	16.02	0.54	0.54
	assign (segid 3A4 and resid 314 and name CB)	(segid 3A4 and resid 390 and name CB)	15.78	0.49	0.49
	assign (segid 3A4 and resid 314 and name CB)	(segid 3A4 and resid 391 and name CA)	15.66	0.56	0.57
	assign (segid 3A4 and resid 314 and name CB)	(segid 3A4 and resid 391 and name CB)	14.46	0.57	0.56
25	assign (segid 3A4 and resid 314 and name CB)	(segid 3A4 and resid 392 and name CA)	18.66	0.57	0.56
	assign (segid 3A4 and resid 314 and name CB)	(segid 3A4 and resid 393 and name CA)	17.59	0.56	0.57
	assign (segid 3A4 and resid 314 and name CB)	(segid 3A4 and resid 394 and name CA)	14.34	0.58	0.59
	assign (segid 3A4 and resid 314 and name CB)	(segid 3A4 and resid 394 and name CB)	13.84	0.67	0.68
30	assign (segid 3A4 and resid 314 and name CB)	(segid 3A4 and resid 395 and name CA)	16.35	0.64	0.64
	assign (segid 3A4 and resid 314 and name CB)	(segid 3A4 and resid 396 and name CA)	17.93	0.58	0.58
	assign (segid 3A4 and resid 314 and name CB)	(segid 3A4 and resid 397 and name CA)	14.85	0.58	0.59
	assign (segid 3A4 and resid 314 and name CB)	(segid 3A4 and resid 397 and name CB)	13.93	0.61	0.60
	assign (segid 3A4 and resid 314 and name CB)	(segid 3A4 and resid 398 and name CA)	13.30	0.54	0.55
	assign (segid 3A4 and resid 314 and name CB)	(segid 3A4 and resid 398 and name CB)	12.94	0.56	0.56
35	assign (segid 3A4 and resid 314 and name CB)	(segid 3A4 and resid 399 and name CA)	16.82	0.53	0.52
	assign (segid 3A4 and resid 314 and name CB)	(segid 3A4 and resid 399 and name CB)	18.06	0.53	0.53
	assign (segid 3A4 and resid 314 and name CB)	(segid 3A4 and resid 400 and name CA)	17.41	0.51	0.51
	assign (segid 3A4 and resid 314 and name CB)	(segid 3A4 and resid 400 and name CB)	17.56	0.48	0.47
40	assign (segid 3A4 and resid 314 and name CB)	(segid 3A4 and resid 401 and name CA)	14.36	0.52	0.51
	assign (segid 3A4 and resid 314 and name CB)	(segid 3A4 and resid 402 and name CA)	15.24	0.43	0.43
	assign (segid 3A4 and resid 314 and name CB)	(segid 3A4 and resid 402 and name CB)	15.30	0.41	0.42
	assign (segid 3A4 and resid 314 and name CB)	(segid 3A4 and resid 403 and name CA)	18.90	0.44	0.44
	assign (segid 3A4 and resid 314 and name CB)	(segid 3A4 and resid 404 and name CA)	18.66	0.55	0.55
45	assign (segid 3A4 and resid 314 and name CB)	(segid 3A4 and resid 404 and name CB)	18.04	0.67	0.66
	assign (segid 3A4 and resid 314 and name CB)	(segid 3A4 and resid 405 and name CA)	16.72	0.35	0.35
	assign (segid 3A4 and resid 314 and name CB)	(segid 3A4 and resid 405 and name CB)	15.27	0.36	0.36
	assign (segid 3A4 and resid 314 and name CB)	(segid 3A4 and resid 406 and name CA)	18.95	0.40	0.40
	assign (segid 3A4 and resid 314 and name CB)	(segid 3A4 and resid 427 and name CA)	18.29	0.92	0.92
50	assign (segid 3A4 and resid 314 and name CB)	(segid 3A4 and resid 431 and name CA)	17.99	0.75	0.74
	assign (segid 3A4 and resid 314 and name CB)	(segid 3A4 and resid 433 and name CA)	14.47	0.51	0.51
	assign (segid 3A4 and resid 314 and name CB)	(segid 3A4 and resid 434 and name CA)	15.23	0.96	0.95
	assign (segid 3A4 and resid 314 and name CB)	(segid 3A4 and resid 435 and name CA)	16.82	1.03	1.04
	assign (segid 3A4 and resid 314 and name CB)	(segid 3A4 and resid 315 and name C)	5.80	0.08	0.09
55	assign (segid 3A4 and resid 314 and name CG)	(segid 3A4 and resid 315 and name CA)	4.71	0.06	0.05
	assign (segid 3A4 and resid 314 and name CG)	(segid 3A4 and resid 315 and name CB)	5.56	0.08	0.08
	assign (segid 3A4 and resid 314 and name CG)	(segid 3A4 and resid 315 and name N)	3.69	0.06	0.05
	assign (segid 3A4 and resid 314 and name CG)	(segid 3A4 and resid 316 and name CA)	6.41	0.16	0.16
	assign (segid 3A4 and resid 314 and name CG)	(segid 3A4 and resid 316 and name N)	7.65	0.10	0.09
60	assign (segid 3A4 and resid 314 and name CG)	(segid 3A4 and resid 317 and name N)	6.42	0.07	0.06
	assign (segid 3A4 and resid 314 and name CG)	(segid 3A4 and resid 348 and name O)	7.17	0.19	0.19
	assign (segid 3A4 and resid 314 and name CG)	(segid 3A4 and resid 350 and name O)	6.67	0.22	0.23
	assign (segid 3A4 and resid 314 and name CG)	(segid 3A4 and resid 350 and name O)	6.59	0.24	0.24
	assign (segid 3A4 and resid 314 and name CG)	(segid 3A4 and resid 351 and name C)	4.40	0.24	0.23
65	assign (segid 3A4 and resid 314 and name CG)	(segid 3A4 and resid 351 and name CA)	4.37	0.22	0.21
	assign (segid 3A4 and resid 314 and name CG)	(segid 3A4 and resid 351 and name N)	5.75	0.23	0.24
	assign (segid 3A4 and resid 314 and name CG)	(segid 3A4 and resid 352 and name O)	3.64	0.24	0.24
	assign (segid 3A4 and resid 314 and name CG)	(segid 3A4 and resid 352 and name C)	7.38	0.34	0.34
	assign (segid 3A4 and resid 314 and name CG)	(segid 3A4 and resid 352 and name CA)	6.26	0.32	0.32
70	assign (segid 3A4 and resid 314 and name CG)	(segid 3A4 and resid 352 and name CB)	7.08	0.31	0.30
	assign (segid 3A4 and resid 314 and name CG)	(segid 3A4 and resid 352 and name CG)	6.55	0.31	0.31
	assign (segid 3A4 and resid 314 and name CG)	(segid 3A4 and resid 352 and name N)	5.61	0.30	0.31
	assign (segid 3A4 and resid 314 and name CG)	(segid 3A4 and resid 353 and name N)	7.48	0.32	0.32
75	assign (segid 3A4 and resid 314 and name CG)	(segid 3A4 and resid 357 and name CA)	7.25	0.31	0.30
	assign (segid 3A4 and resid 314 and name CG)	(segid 3A4 and resid 357 and name CB)	5.82	0.36	0.35
	assign (segid 3A4 and resid 314 and name CG)	(segid 3A4 and resid 360 and name C)	7.12	0.16	0.16
	assign (segid 3A4 and resid 314 and name CG)	(segid 3A4 and resid 360 and name CA)	7.10	0.15	0.14
	assign (segid 3A4 and resid 314 and name CG)	(segid 3A4 and resid 360 and name CB)	7.25	0.22	0.22
80	assign (segid 3A4 and resid 314 and name CG)	(segid 3A4 and resid 360 and name O)	6.20	0.18	0.19
	assign (segid 3A4 and resid 314 and name CG)	(segid 3A4 and resid 362 and name O)	7.51	0.10	0.10
	assign (segid 3A4 and resid 314 and name CG)	(segid 3A4 and resid 381 and name C)	6.55	0.54	0.55
	assign (segid 3A4 and resid 314 and name CG)	(segid 3A4 and resid 381 and name CA)	5.42	0.59	0.58

	assign (segid 3A4 and resid 314 and name CG)	(segid 3A4 and resid 381 and name N)	6.06	0.64	0.64
	assign (segid 3A4 and resid 314 and name CG)	(segid 3A4 and resid 382 and name N)	6.67	0.51	0.51
	assign (segid 3A4 and resid 314 and name N)	(segid 3A4 and resid 314 and name C)	2.46	0.02	0.02
	assign (segid 3A4 and resid 314 and name N)	(segid 3A4 and resid 314 and name CA)	1.46	0.01	0.01
	assign (segid 3A4 and resid 314 and name N)	(segid 3A4 and resid 314 and name CB)	2.48	0.03	0.02
5	assign (segid 3A4 and resid 314 and name N)	(segid 3A4 and resid 314 and name CG)	3.84	0.03	0.03
	assign (segid 3A4 and resid 314 and name N)	(segid 3A4 and resid 314 and name O)	3.45	0.04	0.04
	assign (segid 3A4 and resid 314 and name N)	(segid 3A4 and resid 315 and name C)	4.78	0.06	0.06
	assign (segid 3A4 and resid 314 and name N)	(segid 3A4 and resid 315 and name CA)	4.24	0.04	0.04
	assign (segid 3A4 and resid 314 and name N)	(segid 3A4 and resid 315 and name CB)	5.01	0.09	0.09
10	assign (segid 3A4 and resid 314 and name N)	(segid 3A4 and resid 315 and name N)	2.85	0.05	0.04
	assign (segid 3A4 and resid 314 and name N)	(segid 3A4 and resid 315 and name O)	5.84	0.10	0.10
	assign (segid 3A4 and resid 314 and name N)	(segid 3A4 and resid 316 and name C)	5.49	0.23	0.22
	assign (segid 3A4 and resid 314 and name N)	(segid 3A4 and resid 316 and name CA)	5.57	0.11	0.11
	assign (segid 3A4 and resid 314 and name N)	(segid 3A4 and resid 316 and name N)	4.51	0.08	0.09
15	assign (segid 3A4 and resid 314 and name N)	(segid 3A4 and resid 316 and name O)	6.09	0.65	0.66
	assign (segid 3A4 and resid 314 and name N)	(segid 3A4 and resid 317 and name C)	7.00	0.11	0.12
	assign (segid 3A4 and resid 314 and name N)	(segid 3A4 and resid 317 and name CA)	5.65	0.15	0.15
	assign (segid 3A4 and resid 314 and name N)	(segid 3A4 and resid 317 and name N)	5.16	0.21	0.20
	assign (segid 3A4 and resid 314 and name N)	(segid 3A4 and resid 318 and name N)	7.32	0.23	0.23
20	assign (segid 3A4 and resid 314 and name N)	(segid 3A4 and resid 351 and name C)	7.37	0.23	0.22
	assign (segid 3A4 and resid 314 and name N)	(segid 3A4 and resid 351 and name CA)	6.94	0.17	0.17
	assign (segid 3A4 and resid 314 and name N)	(segid 3A4 and resid 351 and name O)	6.95	0.24	0.24
	assign (segid 3A4 and resid 314 and name N)	(segid 3A4 and resid 381 and name CA)	6.70	0.40	0.41
	assign (segid 3A4 and resid 314 and name N)	(segid 3A4 and resid 382 and name N)	7.25	0.29	0.29
25	assign (segid 3A4 and resid 314 and name N)	(segid 3A4 and resid 383 and name CA)	6.25	0.38	0.39
	assign (segid 3A4 and resid 314 and name N)	(segid 3A4 and resid 383 and name N)	6.46	0.35	0.35
	assign (segid 3A4 and resid 314 and name O)	(segid 3A4 and resid 314 and name CB)	3.37	0.05	0.04
	assign (segid 3A4 and resid 314 and name O)	(segid 3A4 and resid 314 and name CG)	3.45	0.10	0.10
	assign (segid 3A4 and resid 314 and name O)	(segid 3A4 and resid 315 and name C)	3.05	0.07	0.06
30	assign (segid 3A4 and resid 314 and name O)	(segid 3A4 and resid 315 and name CA)	2.79	0.02	0.03
	assign (segid 3A4 and resid 314 and name O)	(segid 3A4 and resid 315 and name CB)	4.28	0.02	0.02
	assign (segid 3A4 and resid 314 and name O)	(segid 3A4 and resid 315 and name N)	2.26	0.01	0.01
	assign (segid 3A4 and resid 314 and name O)	(segid 3A4 and resid 315 and name O)	3.49	0.17	0.16
	assign (segid 3A4 and resid 314 and name O)	(segid 3A4 and resid 316 and name C)	4.54	0.20	0.20
35	assign (segid 3A4 and resid 314 and name O)	(segid 3A4 and resid 316 and name CA)	4.53	0.10	0.11
	assign (segid 3A4 and resid 314 and name O)	(segid 3A4 and resid 316 and name N)	3.59	0.06	0.06
	assign (segid 3A4 and resid 314 and name O)	(segid 3A4 and resid 316 and name O)	5.46	0.31	0.32
	assign (segid 3A4 and resid 314 and name O)	(segid 3A4 and resid 317 and name C)	6.00	0.41	0.42
	assign (segid 3A4 and resid 314 and name O)	(segid 3A4 and resid 317 and name CA)	4.58	0.40	0.41
40	assign (segid 3A4 and resid 314 and name O)	(segid 3A4 and resid 317 and name N)	3.92	0.31	0.32
	assign (segid 3A4 and resid 314 and name O)	(segid 3A4 and resid 317 and name O)	6.55	0.42	0.41
	assign (segid 3A4 and resid 314 and name O)	(segid 3A4 and resid 318 and name N)	6.87	0.46	0.46
	assign (segid 3A4 and resid 314 and name O)	(segid 3A4 and resid 318 and name N)	6.86	0.49	0.50
	assign (segid 3A4 and resid 314 and name O)	(segid 3A4 and resid 347 and name C)	6.18	0.49	0.50
45	assign (segid 3A4 and resid 314 and name O)	(segid 3A4 and resid 347 and name O)	6.15	0.44	0.44
	assign (segid 3A4 and resid 314 and name O)	(segid 3A4 and resid 348 and name C)	5.92	0.46	0.45
	assign (segid 3A4 and resid 314 and name O)	(segid 3A4 and resid 348 and name CA)	6.80	0.51	0.51
	assign (segid 3A4 and resid 314 and name O)	(segid 3A4 and resid 348 and name N)	5.43	0.48	0.48
	assign (segid 3A4 and resid 314 and name O)	(segid 3A4 and resid 348 and name O)	6.95	0.22	0.23
50	assign (segid 3A4 and resid 314 and name O)	(segid 3A4 and resid 350 and name C)	7.41	0.18	0.19
	assign (segid 3A4 and resid 314 and name O)	(segid 3A4 and resid 351 and name C)	4.82	0.23	0.23
	assign (segid 3A4 and resid 314 and name O)	(segid 3A4 and resid 351 and name CA)	4.72	0.19	0.19
	assign (segid 3A4 and resid 314 and name O)	(segid 3A4 and resid 351 and name N)	5.70	0.25	0.24
	assign (segid 3A4 and resid 314 and name O)	(segid 3A4 and resid 351 and name O)	4.63	0.25	0.25
55	assign (segid 3A4 and resid 314 and name O)	(segid 3A4 and resid 352 and name CA)	6.27	0.41	0.41
	assign (segid 3A4 and resid 314 and name O)	(segid 3A4 and resid 352 and name CB)	6.38	0.42	0.41
	assign (segid 3A4 and resid 314 and name O)	(segid 3A4 and resid 352 and name CG)	5.32	0.45	0.44
	assign (segid 3A4 and resid 314 and name O)	(segid 3A4 and resid 352 and name N)	5.59	0.35	0.35
	assign (segid 3A4 and resid 314 and name O)	(segid 3A4 and resid 360 and name O)	6.51	0.30	0.30
60	assign (segid 3A4 and resid 314 and name O)	(segid 3A4 and resid 383 and name CA)	6.93	0.43	0.44
	assign (segid 3A4 and resid 314 and name O)	(segid 3A4 and resid 383 and name N)	7.06	0.43	0.43
	assign (segid 3A4 and resid 314 and name O)	(segid 3A4 and resid 315 and name CB)	2.52	0.03	0.02
	assign (segid 3A4 and resid 315 and name C)	(segid 3A4 and resid 315 and name O)	1.24	0.01	0.01
65	assign (segid 3A4 and resid 315 and name C)	(segid 3A4 and resid 316 and name C)	3.39	0.16	0.15
	assign (segid 3A4 and resid 315 and name C)	(segid 3A4 and resid 316 and name CA)	2.44	0.02	0.02
	assign (segid 3A4 and resid 315 and name C)	(segid 3A4 and resid 316 and name N)	1.34	0.01	0.01
	assign (segid 3A4 and resid 315 and name C)	(segid 3A4 and resid 316 and name O)	4.33	0.19	0.18
	assign (segid 3A4 and resid 315 and name C)	(segid 3A4 and resid 317 and name C)	5.98	0.28	0.28
	assign (segid 3A4 and resid 315 and name C)	(segid 3A4 and resid 317 and name CA)	4.96	0.28	0.27
70	assign (segid 3A4 and resid 315 and name C)	(segid 3A4 and resid 317 and name N)	3.63	0.26	0.26
	assign (segid 3A4 and resid 315 and name C)	(segid 3A4 and resid 317 and name O)	6.35	0.39	0.38
	assign (segid 3A4 and resid 315 and name C)	(segid 3A4 and resid 318 and name N)	6.76	0.36	0.36
	assign (segid 3A4 and resid 315 and name C)	(segid 3A4 and resid 351 and name C)	7.18	0.25	0.25
75	assign (segid 3A4 and resid 315 and name C)	(segid 3A4 and resid 351 and name CA)	7.44	0.28	0.27
	assign (segid 3A4 and resid 315 and name C)	(segid 3A4 and resid 351 and name O)	6.85	0.22	0.23
	assign (segid 3A4 and resid 315 and name C)	(segid 3A4 and resid 352 and name CG)	6.12	0.40	0.40
	assign (segid 3A4 and resid 315 and name C)	(segid 3A4 and resid 360 and name O)	6.55	0.30	0.30
	assign (segid 3A4 and resid 315 and name C)	(segid 3A4 and resid 315 and name C)	1.51	0.02	0.02
80	assign (segid 3A4 and resid 315 and name CA)	(segid 3A4 and resid 315 and name CB)	1.54	0.02	0.03
	assign (segid 3A4 and resid 315 and name CA)	(segid 3A4 and resid 315 and name O)	2.38	0.02	0.01
	assign (segid 3A4 and resid 315 and name CA)	(segid 3A4 and resid 316 and name C)	4.66	0.10	0.09
	assign (segid 3A4 and resid 315 and name CA)	(segid 3A4 and resid 316 and name CA)	3.82	0.02	0.02

	assign (segid 3A4 and resid 315 and name CA)	(segid 3A4 and resid 316 and name N)	2.46	0.02	0.02
	assign (segid 3A4 and resid 315 and name CA)	(segid 3A4 and resid 316 and name O)	5.55	0.17	0.17
	assign (segid 3A4 and resid 315 and name CA)	(segid 3A4 and resid 317 and name C)	7.14	0.30	0.30
	assign (segid 3A4 and resid 315 and name CA)	(segid 3A4 and resid 317 and name CA)	5.95	0.29	0.29
5	assign (segid 3A4 and resid 315 and name CA)	(segid 3A4 and resid 317 and name N)	4.75	0.29	0.30
	assign (segid 3A4 and resid 315 and name CA)	(segid 3A4 and resid 318 and name CA)	9.08	0.29	0.30
	assign (segid 3A4 and resid 315 and name CA)	(segid 3A4 and resid 318 and name CB)	9.59	0.38	0.37
	assign (segid 3A4 and resid 315 and name CA)	(segid 3A4 and resid 319 and name CA)	11.64	0.28	0.28
	assign (segid 3A4 and resid 315 and name CA)	(segid 3A4 and resid 319 and name CB)	12.35	0.22	0.23
10	assign (segid 3A4 and resid 315 and name CA)	(segid 3A4 and resid 344 and name CA)	19.21	0.41	0.42
	assign (segid 3A4 and resid 315 and name CA)	(segid 3A4 and resid 344 and name CB)	19.08	0.37	0.38
	assign (segid 3A4 and resid 315 and name CA)	(segid 3A4 and resid 345 and name CA)	16.45	0.58	0.58
	assign (segid 3A4 and resid 315 and name CA)	(segid 3A4 and resid 345 and name CB)	16.65	0.76	0.75
	assign (segid 3A4 and resid 315 and name CA)	(segid 3A4 and resid 346 and name CA)	13.29	0.50	0.49
	assign (segid 3A4 and resid 315 and name CA)	(segid 3A4 and resid 346 and name CB)	13.37	0.46	0.46
15	assign (segid 3A4 and resid 315 and name CA)	(segid 3A4 and resid 347 and name CA)	10.71	0.58	0.59
	assign (segid 3A4 and resid 315 and name CA)	(segid 3A4 and resid 347 and name CB)	10.72	0.61	0.62
	assign (segid 3A4 and resid 315 and name CA)	(segid 3A4 and resid 348 and name CA)	7.97	0.63	0.64
	assign (segid 3A4 and resid 315 and name CA)	(segid 3A4 and resid 349 and name CA)	9.97	0.65	0.65
	assign (segid 3A4 and resid 315 and name CA)	(segid 3A4 and resid 349 and name CB)	11.42	0.67	0.67
20	assign (segid 3A4 and resid 315 and name CA)	(segid 3A4 and resid 350 and name CA)	10.40	0.33	0.33
	assign (segid 3A4 and resid 315 and name CA)	(segid 3A4 and resid 350 and name CB)	10.99	0.36	0.36
	assign (segid 3A4 and resid 315 and name CA)	(segid 3A4 and resid 351 and name C)	6.63	0.19	0.18
	assign (segid 3A4 and resid 315 and name CA)	(segid 3A4 and resid 351 and name CA)	7.00	0.21	0.20
	assign (segid 3A4 and resid 315 and name CA)	(segid 3A4 and resid 351 and name O)	6.08	0.15	0.14
25	assign (segid 3A4 and resid 315 and name CA)	(segid 3A4 and resid 352 and name CA)	7.42	0.33	0.32
	assign (segid 3A4 and resid 315 and name CA)	(segid 3A4 and resid 352 and name CB)	7.28	0.29	0.28
	assign (segid 3A4 and resid 315 and name CA)	(segid 3A4 and resid 352 and name CG)	6.01	0.21	0.21
	assign (segid 3A4 and resid 315 and name CA)	(segid 3A4 and resid 352 and name N)	7.24	0.30	0.29
	assign (segid 3A4 and resid 315 and name CA)	(segid 3A4 and resid 353 and name CA)	11.02	0.32	0.31
30	assign (segid 3A4 and resid 315 and name CA)	(segid 3A4 and resid 353 and name CB)	11.77	0.29	0.29
	assign (segid 3A4 and resid 315 and name CA)	(segid 3A4 and resid 354 and name CA)	12.60	0.42	0.43
	assign (segid 3A4 and resid 315 and name CA)	(segid 3A4 and resid 354 and name CB)	13.47	0.49	0.48
	assign (segid 3A4 and resid 315 and name CA)	(segid 3A4 and resid 355 and name CA)	15.17	0.37	0.37
	assign (segid 3A4 and resid 315 and name CA)	(segid 3A4 and resid 355 and name CB)	16.09	0.34	0.33
35	assign (segid 3A4 and resid 315 and name CA)	(segid 3A4 and resid 356 and name CA)	13.07	0.40	0.40
	assign (segid 3A4 and resid 315 and name CA)	(segid 3A4 and resid 356 and name CB)	12.47	0.43	0.43
	assign (segid 3A4 and resid 315 and name CA)	(segid 3A4 and resid 357 and name CA)	10.53	0.39	0.40
	assign (segid 3A4 and resid 315 and name CA)	(segid 3A4 and resid 357 and name CB)	9.04	0.39	0.38
	assign (segid 3A4 and resid 315 and name CA)	(segid 3A4 and resid 358 and name CA)	12.44	0.39	0.39
40	assign (segid 3A4 and resid 315 and name CA)	(segid 3A4 and resid 358 and name CB)	13.53	0.54	0.55
	assign (segid 3A4 and resid 315 and name CA)	(segid 3A4 and resid 359 and name CA)	10.99	0.21	0.22
	assign (segid 3A4 and resid 315 and name CA)	(segid 3A4 and resid 359 and name CB)	11.53	0.22	0.22
	assign (segid 3A4 and resid 315 and name CA)	(segid 3A4 and resid 360 and name C)	6.82	0.21	0.21
	assign (segid 3A4 and resid 315 and name CA)	(segid 3A4 and resid 360 and name CA)	7.72	0.23	0.23
45	assign (segid 3A4 and resid 315 and name CA)	(segid 3A4 and resid 360 and name CB)	8.18	0.28	0.28
	assign (segid 3A4 and resid 315 and name CA)	(segid 3A4 and resid 361 and name C)	5.60	0.21	0.21
	assign (segid 3A4 and resid 315 and name CA)	(segid 3A4 and resid 361 and name CA)	7.23	0.19	0.20
	assign (segid 3A4 and resid 315 and name CA)	(segid 3A4 and resid 361 and name CB)	8.38	0.24	0.24
50	assign (segid 3A4 and resid 315 and name CA)	(segid 3A4 and resid 361 and name N)	7.58	0.22	0.21
	assign (segid 3A4 and resid 315 and name CA)	(segid 3A4 and resid 361 and name O)	7.28	0.35	0.35
	assign (segid 3A4 and resid 315 and name CA)	(segid 3A4 and resid 362 and name C)	7.08	0.26	0.25
	assign (segid 3A4 and resid 315 and name CA)	(segid 3A4 and resid 362 and name CA)	8.01	0.23	0.22
	assign (segid 3A4 and resid 315 and name CA)	(segid 3A4 and resid 362 and name CB)	9.31	0.25	0.24
55	assign (segid 3A4 and resid 315 and name CA)	(segid 3A4 and resid 362 and name N)	7.58	0.19	0.20
	assign (segid 3A4 and resid 315 and name CA)	(segid 3A4 and resid 362 and name O)	6.59	0.21	0.22
	assign (segid 3A4 and resid 315 and name CA)	(segid 3A4 and resid 363 and name CA)	6.68	0.42	0.42
	assign (segid 3A4 and resid 315 and name CA)	(segid 3A4 and resid 363 and name CB)	6.76	0.46	0.47
	assign (segid 3A4 and resid 315 and name CA)	(segid 3A4 and resid 363 and name CG)	6.76	0.47	0.47
60	assign (segid 3A4 and resid 315 and name CA)	(segid 3A4 and resid 364 and name CA)	9.18	0.37	0.38
	assign (segid 3A4 and resid 315 and name CA)	(segid 3A4 and resid 364 and name CB)	9.87	0.36	0.35
	assign (segid 3A4 and resid 315 and name CA)	(segid 3A4 and resid 365 and name CA)	10.27	0.32	0.31
	assign (segid 3A4 and resid 315 and name CA)	(segid 3A4 and resid 365 and name CB)	11.05	0.27	0.27
65	assign (segid 3A4 and resid 315 and name CA)	(segid 3A4 and resid 381 and name CA)	9.49	0.53	0.52
	assign (segid 3A4 and resid 315 and name CA)	(segid 3A4 and resid 382 and name CA)	10.91	0.39	0.39
	assign (segid 3A4 and resid 315 and name CA)	(segid 3A4 and resid 382 and name CB)	11.65	0.46	0.46
	assign (segid 3A4 and resid 315 and name CA)	(segid 3A4 and resid 383 and name CA)	9.27	0.38	0.38
	assign (segid 3A4 and resid 315 and name CA)	(segid 3A4 and resid 384 and name CA)	12.84	0.40	0.41
70	assign (segid 3A4 and resid 315 and name CA)	(segid 3A4 and resid 385 and name CA)	13.42	0.44	0.44
	assign (segid 3A4 and resid 315 and name CA)	(segid 3A4 and resid 386 and name CA)	14.57	0.36	0.36
	assign (segid 3A4 and resid 315 and name CA)	(segid 3A4 and resid 386 and name CB)	17.11	0.43	0.44
	assign (segid 3A4 and resid 315 and name CA)	(segid 3A4 and resid 390 and name CA)	18.56	0.34	0.33
	assign (segid 3A4 and resid 315 and name CA)	(segid 3A4 and resid 390 and name CB)	18.60	0.34	0.35
75	assign (segid 3A4 and resid 315 and name CA)	(segid 3A4 and resid 391 and name CA)	17.75	0.35	0.35
	assign (segid 3A4 and resid 315 and name CA)	(segid 3A4 and resid 391 and name CB)	16.43	0.36	0.37
	assign (segid 3A4 and resid 315 and name CA)	(segid 3A4 and resid 394 and name CA)	16.62	0.48	0.48
	assign (segid 3A4 and resid 315 and name CA)	(segid 3A4 and resid 394 and name CB)	16.42	0.59	0.60
	assign (segid 3A4 and resid 315 and name CA)	(segid 3A4 and resid 395 and name CA)	18.82	0.55	0.56
	assign (segid 3A4 and resid 315 and name CA)	(segid 3A4 and resid 397 and name CA)	16.15	0.52	0.52
80	assign (segid 3A4 and resid 315 and name CA)	(segid 3A4 and resid 397 and name CB)	15.23	0.53	0.54
	assign (segid 3A4 and resid 315 and name CA)	(segid 3A4 and resid 398 and name CA)	15.15	0.51	0.51
	assign (segid 3A4 and resid 315 and name CA)	(segid 3A4 and resid 398 and name CB)	15.19	0.53	0.53

	assign (segid 3A4 and resid 315 and name CA) (segid 3A4 and resid 399 and name CA)	18.47	0.51	0.52
	assign (segid 3A4 and resid 315 and name CA) (segid 3A4 and resid 400 and name CA)	18.20	0.56	0.57
	assign (segid 3A4 and resid 315 and name CA) (segid 3A4 and resid 400 and name CB)	18.19	0.54	0.54
	assign (segid 3A4 and resid 315 and name CA) (segid 3A4 and resid 401 and name CA)	14.87	0.59	0.58
	assign (segid 3A4 and resid 315 and name CA) (segid 3A4 and resid 402 and name CA)	16.30	0.50	0.50
5	assign (segid 3A4 and resid 315 and name CA) (segid 3A4 and resid 402 and name CB)	16.75	0.46	0.47
	assign (segid 3A4 and resid 315 and name CA) (segid 3A4 and resid 404 and name CB)	17.77	0.85	0.85
	assign (segid 3A4 and resid 315 and name CA) (segid 3A4 and resid 405 and name CA)	16.49	0.50	0.50
	assign (segid 3A4 and resid 315 and name CA) (segid 3A4 and resid 405 and name CB)	15.13	0.50	0.51
	assign (segid 3A4 and resid 315 and name CA) (segid 3A4 and resid 425 and name CA)	15.42	2.23	2.22
10	assign (segid 3A4 and resid 315 and name CA) (segid 3A4 and resid 426 and name CA)	14.29	1.64	1.64
	assign (segid 3A4 and resid 315 and name CA) (segid 3A4 and resid 427 and name CA)	14.76	1.14	1.14
	assign (segid 3A4 and resid 315 and name CA) (segid 3A4 and resid 428 and name CA)	16.32	1.16	1.16
	assign (segid 3A4 and resid 315 and name CA) (segid 3A4 and resid 429 and name CA)	16.22	0.56	0.57
	assign (segid 3A4 and resid 315 and name CA) (segid 3A4 and resid 430 and name CA)	16.92	0.82	0.82
15	assign (segid 3A4 and resid 315 and name CA) (segid 3A4 and resid 431 and name CA)	16.33	0.45	0.46
	assign (segid 3A4 and resid 315 and name CA) (segid 3A4 and resid 433 and name CA)	11.79	0.69	0.69
	assign (segid 3A4 and resid 315 and name CA) (segid 3A4 and resid 434 and name CA)	12.24	0.93	0.94
	assign (segid 3A4 and resid 315 and name CA) (segid 3A4 and resid 435 and name CA)	13.41	1.10	1.11
	assign (segid 3A4 and resid 315 and name CA) (segid 3A4 and resid 436 and name CA)	16.99	1.26	1.26
20	assign (segid 3A4 and resid 315 and name CA) (segid 3A4 and resid 438 and name CA)	17.77	0.96	0.96
	assign (segid 3A4 and resid 315 and name CB) (segid 3A4 and resid 316 and name C)	5.59	0.09	0.10
	assign (segid 3A4 and resid 315 and name CB) (segid 3A4 and resid 316 and name CA)	4.51	0.05	0.06
	assign (segid 3A4 and resid 315 and name CB) (segid 3A4 and resid 316 and name N)	3.19	0.07	0.07
	assign (segid 3A4 and resid 315 and name CB) (segid 3A4 and resid 316 and name O)	6.37	0.26	0.27
25	assign (segid 3A4 and resid 315 and name CB) (segid 3A4 and resid 317 and name CA)	7.21	0.19	0.19
	assign (segid 3A4 and resid 315 and name CB) (segid 3A4 and resid 317 and name N)	5.94	0.21	0.21
	assign (segid 3A4 and resid 315 and name CB) (segid 3A4 and resid 318 and name CA)	10.06	0.20	0.21
	assign (segid 3A4 and resid 315 and name CB) (segid 3A4 and resid 318 and name CB)	10.43	0.25	0.25
30	assign (segid 3A4 and resid 315 and name CB) (segid 3A4 and resid 319 and name CA)	12.87	0.28	0.29
	assign (segid 3A4 and resid 315 and name CB) (segid 3A4 and resid 319 and name CB)	13.60	0.22	0.22
	assign (segid 3A4 and resid 315 and name CB) (segid 3A4 and resid 345 and name CA)	17.97	0.59	0.60
	assign (segid 3A4 and resid 315 and name CB) (segid 3A4 and resid 345 and name CB)	18.17	0.77	0.77
	assign (segid 3A4 and resid 315 and name CB) (segid 3A4 and resid 346 and name CA)	14.77	0.52	0.52
35	assign (segid 3A4 and resid 315 and name CB) (segid 3A4 and resid 346 and name CB)	14.82	0.48	0.48
	assign (segid 3A4 and resid 315 and name CB) (segid 3A4 and resid 347 and name CA)	12.24	0.60	0.61
	assign (segid 3A4 and resid 315 and name CB) (segid 3A4 and resid 347 and name CB)	12.24	0.64	0.64
	assign (segid 3A4 and resid 315 and name CB) (segid 3A4 and resid 348 and name CA)	9.45	0.68	0.67
	assign (segid 3A4 and resid 315 and name CB) (segid 3A4 and resid 349 and name CA)	11.32	0.66	0.67
	assign (segid 3A4 and resid 315 and name CB) (segid 3A4 and resid 349 and name CB)	12.76	0.69	0.70
40	assign (segid 3A4 and resid 315 and name CB) (segid 3A4 and resid 350 and name CA)	11.78	0.32	0.31
	assign (segid 3A4 and resid 315 and name CB) (segid 3A4 and resid 350 and name CB)	12.41	0.35	0.35
	assign (segid 3A4 and resid 315 and name CB) (segid 3A4 and resid 351 and name CA)	8.30	0.21	0.21
	assign (segid 3A4 and resid 315 and name CB) (segid 3A4 and resid 351 and name O)	7.10	0.15	0.14
	assign (segid 3A4 and resid 315 and name CB) (segid 3A4 and resid 352 and name CA)	8.41	0.33	0.33
45	assign (segid 3A4 and resid 315 and name CB) (segid 3A4 and resid 352 and name CB)	8.26	0.28	0.27
	assign (segid 3A4 and resid 315 and name CB) (segid 3A4 and resid 352 and name CG)	7.01	0.17	0.18
	assign (segid 3A4 and resid 315 and name CB) (segid 3A4 and resid 353 and name CA)	11.96	0.34	0.35
	assign (segid 3A4 and resid 315 and name CB) (segid 3A4 and resid 353 and name CB)	12.81	0.32	0.32
	assign (segid 3A4 and resid 315 and name CB) (segid 3A4 and resid 354 and name CA)	13.17	0.48	0.49
50	assign (segid 3A4 and resid 315 and name CB) (segid 3A4 and resid 354 and name CB)	13.97	0.56	0.56
	assign (segid 3A4 and resid 315 and name CB) (segid 3A4 and resid 355 and name CA)	15.85	0.44	0.44
	assign (segid 3A4 and resid 315 and name CB) (segid 3A4 and resid 355 and name CB)	16.86	0.39	0.38
	assign (segid 3A4 and resid 315 and name CB) (segid 3A4 and resid 356 and name CA)	13.77	0.42	0.43
	assign (segid 3A4 and resid 315 and name CB) (segid 3A4 and resid 356 and name CB)	13.31	0.45	0.46
55	assign (segid 3A4 and resid 315 and name CB) (segid 3A4 and resid 357 and name CA)	10.93	0.42	0.43
	assign (segid 3A4 and resid 315 and name CB) (segid 3A4 and resid 357 and name CB)	9.48	0.41	0.42
	assign (segid 3A4 and resid 315 and name CB) (segid 3A4 and resid 358 and name CA)	12.45	0.39	0.39
	assign (segid 3A4 and resid 315 and name CB) (segid 3A4 and resid 358 and name CB)	13.45	0.57	0.57
	assign (segid 3A4 and resid 315 and name CB) (segid 3A4 and resid 359 and name CA)	10.74	0.29	0.28
60	assign (segid 3A4 and resid 315 and name CB) (segid 3A4 and resid 359 and name CB)	11.09	0.30	0.30
	assign (segid 3A4 and resid 315 and name CB) (segid 3A4 and resid 360 and name C)	6.81	0.29	0.28
	assign (segid 3A4 and resid 315 and name CB) (segid 3A4 and resid 360 and name CA)	7.83	0.27	0.27
	assign (segid 3A4 and resid 315 and name CB) (segid 3A4 and resid 360 and name CB)	8.54	0.28	0.29
	assign (segid 3A4 and resid 315 and name CB) (segid 3A4 and resid 360 and name O)	5.61	0.29	0.30
65	assign (segid 3A4 and resid 315 and name CB) (segid 3A4 and resid 361 and name C)	6.68	0.32	0.32
	assign (segid 3A4 and resid 315 and name CB) (segid 3A4 and resid 361 and name CA)	6.95	0.34	0.34
	assign (segid 3A4 and resid 315 and name CB) (segid 3A4 and resid 361 and name CB)	8.14	0.39	0.39
	assign (segid 3A4 and resid 315 and name CB) (segid 3A4 and resid 361 and name N)	7.43	0.32	0.33
	assign (segid 3A4 and resid 315 and name CB) (segid 3A4 and resid 361 and name O)	6.55	0.48	0.47
70	assign (segid 3A4 and resid 315 and name CB) (segid 3A4 and resid 362 and name C)	6.05	0.26	0.27
	assign (segid 3A4 and resid 315 and name CB) (segid 3A4 and resid 362 and name CA)	7.10	0.25	0.25
	assign (segid 3A4 and resid 315 and name CB) (segid 3A4 and resid 362 and name CB)	8.41	0.26	0.26
	assign (segid 3A4 and resid 315 and name CB) (segid 3A4 and resid 362 and name N)	6.92	0.25	0.25
	assign (segid 3A4 and resid 315 and name CB) (segid 3A4 and resid 362 and name O)	5.71	0.25	0.25
75	assign (segid 3A4 and resid 315 and name CB) (segid 3A4 and resid 363 and name C)	6.57	0.43	0.43
	assign (segid 3A4 and resid 315 and name CB) (segid 3A4 and resid 363 and name CA)	5.35	0.43	0.43
	assign (segid 3A4 and resid 315 and name CB) (segid 3A4 and resid 363 and name CB)	5.30	0.48	0.48
	assign (segid 3A4 and resid 315 and name CB) (segid 3A4 and resid 363 and name CG)	5.28	0.52	0.51
	assign (segid 3A4 and resid 315 and name CB) (segid 3A4 and resid 363 and name N)	5.90	0.35	0.36
80	assign (segid 3A4 and resid 315 and name CB) (segid 3A4 and resid 364 and name CA)	8.05	0.42	0.43
	assign (segid 3A4 and resid 315 and name CB) (segid 3A4 and resid 364 and name CB)	8.85	0.41	0.40
	assign (segid 3A4 and resid 315 and name CB) (segid 3A4 and resid 364 and name N)	6.71	0.43	0.44

	assign (segid 3A4 and resid 315 and name CB)	(segid 3A4 and resid 365 and name CA)	9.26	0.38	0.39
	assign (segid 3A4 and resid 315 and name CB)	(segid 3A4 and resid 365 and name CB)	9.98	0.37	0.36
	assign (segid 3A4 and resid 315 and name CB)	(segid 3A4 and resid 381 and name CA)	10.58	0.53	0.53
	assign (segid 3A4 and resid 315 and name CB)	(segid 3A4 and resid 382 and name CA)	12.24	0.40	0.40
	assign (segid 3A4 and resid 315 and name CB)	(segid 3A4 and resid 382 and name CB)	13.05	0.47	0.47
5	assign (segid 3A4 and resid 315 and name CB)	(segid 3A4 and resid 383 and name CA)	10.55	0.40	0.41
	assign (segid 3A4 and resid 315 and name CB)	(segid 3A4 and resid 384 and name CA)	14.01	0.44	0.44
	assign (segid 3A4 and resid 315 and name CB)	(segid 3A4 and resid 384 and name CB)	14.49	0.49	0.49
	assign (segid 3A4 and resid 315 and name CB)	(segid 3A4 and resid 385 and name CA)	15.92	0.38	0.39
	assign (segid 3A4 and resid 315 and name CB)	(segid 3A4 and resid 386 and name CA)	18.45	0.46	0.46
10	assign (segid 3A4 and resid 315 and name CB)	(segid 3A4 and resid 391 and name CA)	18.85	0.41	0.40
	assign (segid 3A4 and resid 315 and name CB)	(segid 3A4 and resid 391 and name CB)	17.48	0.41	0.42
	assign (segid 3A4 and resid 315 and name CB)	(segid 3A4 and resid 394 and name CA)	17.36	0.53	0.52
	assign (segid 3A4 and resid 315 and name CB)	(segid 3A4 and resid 394 and name CB)	17.22	0.62	0.63
	assign (segid 3A4 and resid 315 and name CB)	(segid 3A4 and resid 397 and name CA)	16.55	0.57	0.57
15	assign (segid 3A4 and resid 315 and name CB)	(segid 3A4 and resid 397 and name CB)	15.74	0.57	0.58
	assign (segid 3A4 and resid 315 and name CB)	(segid 3A4 and resid 398 and name CA)	15.35	0.56	0.57
	assign (segid 3A4 and resid 315 and name CB)	(segid 3A4 and resid 398 and name CB)	15.44	0.59	0.59
	assign (segid 3A4 and resid 315 and name CB)	(segid 3A4 and resid 399 and name CA)	18.51	0.56	0.56
	assign (segid 3A4 and resid 315 and name CB)	(segid 3A4 and resid 399 and name CB)	18.17	0.60	0.59
20	assign (segid 3A4 and resid 315 and name CB)	(segid 3A4 and resid 400 and name CA)	18.25	0.56	0.56
	assign (segid 3A4 and resid 315 and name CB)	(segid 3A4 and resid 400 and name CB)	14.68	0.62	0.62
	assign (segid 3A4 and resid 315 and name CB)	(segid 3A4 and resid 401 and name CA)	15.92	0.56	0.56
	assign (segid 3A4 and resid 315 and name CB)	(segid 3A4 and resid 402 and name CA)	16.44	0.52	0.52
	assign (segid 3A4 and resid 315 and name CB)	(segid 3A4 and resid 402 and name CB)	18.06	0.76	0.76
25	assign (segid 3A4 and resid 315 and name CB)	(segid 3A4 and resid 404 and name CA)	17.32	0.88	0.89
	assign (segid 3A4 and resid 315 and name CB)	(segid 3A4 and resid 404 and name CB)	15.75	0.55	0.55
	assign (segid 3A4 and resid 315 and name CB)	(segid 3A4 and resid 405 and name CA)	14.40	0.58	0.57
	assign (segid 3A4 and resid 315 and name CB)	(segid 3A4 and resid 405 and name CB)	18.45	0.51	0.52
	assign (segid 3A4 and resid 315 and name CB)	(segid 3A4 and resid 406 and name CA)	18.43	0.48	0.48
30	assign (segid 3A4 and resid 315 and name CB)	(segid 3A4 and resid 408 and name CB)	17.95	0.63	0.63
	assign (segid 3A4 and resid 315 and name CB)	(segid 3A4 and resid 409 and name CA)	15.38	2.43	2.43
	assign (segid 3A4 and resid 315 and name CB)	(segid 3A4 and resid 424 and name CA)	15.06	2.28	2.28
	assign (segid 3A4 and resid 315 and name CB)	(segid 3A4 and resid 425 and name CA)	14.27	1.59	1.58
	assign (segid 3A4 and resid 315 and name CB)	(segid 3A4 and resid 426 and name CA)	15.03	1.23	1.23
35	assign (segid 3A4 and resid 315 and name CB)	(segid 3A4 and resid 427 and name CA)	16.83	1.15	1.15
	assign (segid 3A4 and resid 315 and name CB)	(segid 3A4 and resid 428 and name CA)	16.96	0.63	0.62
	assign (segid 3A4 and resid 315 and name CB)	(segid 3A4 and resid 429 and name CA)	17.88	0.77	0.78
	assign (segid 3A4 and resid 315 and name CB)	(segid 3A4 and resid 430 and name CA)	17.40	0.43	0.44
	assign (segid 3A4 and resid 315 and name CB)	(segid 3A4 and resid 431 and name CA)	12.49	0.79	0.79
40	assign (segid 3A4 and resid 315 and name CB)	(segid 3A4 and resid 433 and name CA)	12.57	0.96	0.95
	assign (segid 3A4 and resid 315 and name CB)	(segid 3A4 and resid 434 and name CA)	13.33	1.13	1.13
	assign (segid 3A4 and resid 315 and name CB)	(segid 3A4 and resid 435 and name CA)	16.88	1.34	1.33
	assign (segid 3A4 and resid 315 and name CB)	(segid 3A4 and resid 436 and name CA)	18.35	0.96	0.96
	assign (segid 3A4 and resid 315 and name CB)	(segid 3A4 and resid 437 and name CA)	17.13	0.99	0.99
45	assign (segid 3A4 and resid 315 and name CB)	(segid 3A4 and resid 438 and name CA)	2.48	0.03	0.04
	assign (segid 3A4 and resid 315 and name N)	(segid 3A4 and resid 315 and name C)	1.45	0.00	0.01
	assign (segid 3A4 and resid 315 and name N)	(segid 3A4 and resid 315 and name CA)	2.44	0.02	0.02
	assign (segid 3A4 and resid 315 and name N)	(segid 3A4 and resid 315 and name CB)	3.50	0.06	0.06
	assign (segid 3A4 and resid 315 and name N)	(segid 3A4 and resid 315 and name O)	4.84	0.08	0.09
50	assign (segid 3A4 and resid 315 and name N)	(segid 3A4 and resid 316 and name CA)	4.32	0.04	0.05
	assign (segid 3A4 and resid 315 and name N)	(segid 3A4 and resid 316 and name N)	2.93	0.04	0.03
	assign (segid 3A4 and resid 315 and name N)	(segid 3A4 and resid 316 and name O)	5.70	0.31	0.31
	assign (segid 3A4 and resid 315 and name N)	(segid 3A4 and resid 316 and name C)	7.08	0.23	0.23
	assign (segid 3A4 and resid 315 and name N)	(segid 3A4 and resid 317 and name CA)	5.75	0.22	0.22
55	assign (segid 3A4 and resid 315 and name N)	(segid 3A4 and resid 317 and name N)	4.74	0.27	0.27
	assign (segid 3A4 and resid 315 and name N)	(segid 3A4 and resid 351 and name C)	6.39	0.16	0.17
	assign (segid 3A4 and resid 315 and name N)	(segid 3A4 and resid 351 and name CA)	6.53	0.15	0.15
	assign (segid 3A4 and resid 315 and name N)	(segid 3A4 and resid 351 and name O)	5.82	0.15	0.15
	assign (segid 3A4 and resid 315 and name N)	(segid 3A4 and resid 352 and name CG)	6.59	0.22	0.22
60	assign (segid 3A4 and resid 315 and name N)	(segid 3A4 and resid 352 and name N)	7.22	0.27	0.28
	assign (segid 3A4 and resid 315 and name N)	(segid 3A4 and resid 360 and name C)	7.45	0.18	0.18
	assign (segid 3A4 and resid 315 and name N)	(segid 3A4 and resid 360 and name O)	6.24	0.18	0.19
	assign (segid 3A4 and resid 315 and name N)	(segid 3A4 and resid 362 and name C)	7.71	0.14	0.15
	assign (segid 3A4 and resid 315 and name N)	(segid 3A4 and resid 362 and name O)	7.06	0.11	0.10
65	assign (segid 3A4 and resid 315 and name N)	(segid 3A4 and resid 363 and name CA)	7.19	0.25	0.24
	assign (segid 3A4 and resid 315 and name N)	(segid 3A4 and resid 363 and name CG)	7.16	0.31	0.30
	assign (segid 3A4 and resid 315 and name N)	(segid 3A4 and resid 315 and name CB)	3.30	0.06	0.07
	assign (segid 3A4 and resid 315 and name O)	(segid 3A4 and resid 316 and name C)	3.62	0.29	0.30
	assign (segid 3A4 and resid 315 and name O)	(segid 3A4 and resid 316 and name CA)	2.76	0.05	0.04
70	assign (segid 3A4 and resid 315 and name O)	(segid 3A4 and resid 316 and name N)	2.25	0.01	0.01
	assign (segid 3A4 and resid 315 and name O)	(segid 3A4 and resid 316 and name O)	4.53	0.46	0.46
	assign (segid 3A4 and resid 315 and name O)	(segid 3A4 and resid 317 and name C)	5.98	0.39	0.40
	assign (segid 3A4 and resid 315 and name O)	(segid 3A4 and resid 317 and name CA)	5.09	0.39	0.40
	assign (segid 3A4 and resid 315 and name O)	(segid 3A4 and resid 317 and name N)	3.82	0.28	0.29
75	assign (segid 3A4 and resid 315 and name O)	(segid 3A4 and resid 317 and name O)	6.12	0.46	0.47
	assign (segid 3A4 and resid 315 and name O)	(segid 3A4 and resid 318 and name N)	6.91	0.45	0.44
	assign (segid 3A4 and resid 315 and name O)	(segid 3A4 and resid 351 and name C)	7.01	0.34	0.35
	assign (segid 3A4 and resid 315 and name O)	(segid 3A4 and resid 351 and name CA)	7.38	0.38	0.39
80	assign (segid 3A4 and resid 315 and name O)	(segid 3A4 and resid 351 and name O)	6.80	0.33	0.34
	assign (segid 3A4 and resid 315 and name O)	(segid 3A4 and resid 352 and name CB)	6.82	0.47	0.47
	assign (segid 3A4 and resid 315 and name O)	(segid 3A4 and resid 352 and name CG)	5.40	0.48	0.48
	assign (segid 3A4 and resid 315 and name O)	(segid 3A4 and resid 352 and name N)	7.27	0.39	0.40

	assign (segid 3A4 and resid 315 and name O)	(segid 3A4 and resid 360 and name O)	6.34	0.39	0.38
	assign (segid 3A4 and resid 316 and name C)	(segid 3A4 and resid 316 and name O)	1.23	0.01	0.00
	assign (segid 3A4 and resid 316 and name C)	(segid 3A4 and resid 317 and name C)	2.99	0.09	0.09
	assign (segid 3A4 and resid 316 and name C)	(segid 3A4 and resid 317 and name CA)	2.46	0.01	0.00
5	assign (segid 3A4 and resid 316 and name C)	(segid 3A4 and resid 317 and name N)	1.33	0.00	0.01
	assign (segid 3A4 and resid 316 and name C)	(segid 3A4 and resid 317 and name O)	3.53	0.25	0.25
	assign (segid 3A4 and resid 316 and name C)	(segid 3A4 and resid 318 and name C)	5.82	0.21	0.22
	assign (segid 3A4 and resid 316 and name C)	(segid 3A4 and resid 318 and name CA)	4.61	0.18	0.19
	assign (segid 3A4 and resid 316 and name C)	(segid 3A4 and resid 318 and name CB)	5.19	0.30	0.30
	assign (segid 3A4 and resid 316 and name C)	(segid 3A4 and resid 318 and name N)	3.59	0.23	0.23
10	assign (segid 3A4 and resid 316 and name C)	(segid 3A4 and resid 318 and name O)	6.62	0.25	0.26
	assign (segid 3A4 and resid 316 and name C)	(segid 3A4 and resid 319 and name N)	6.25	0.23	0.24
	assign (segid 3A4 and resid 316 and name C)	(segid 3A4 and resid 348 and name CA)	6.82	0.48	0.48
	assign (segid 3A4 and resid 316 and name C)	(segid 3A4 and resid 316 and name C)	1.53	0.02	0.01
	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 316 and name O)	2.39	0.03	0.02
15	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 317 and name C)	4.38	0.06	0.07
	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 317 and name CA)	3.83	0.02	0.02
	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 317 and name N)	2.44	0.02	0.02
	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 317 and name O)	4.76	0.29	0.30
	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 318 and name C)	7.12	0.25	0.24
20	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 318 and name CA)	5.85	0.27	0.27
	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 318 and name CB)	6.30	0.41	0.42
	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 318 and name N)	4.95	0.30	0.31
	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 319 and name CA)	8.94	0.31	0.30
	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 319 and name CB)	9.83	0.19	0.19
25	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 322 and name CA)	18.86	0.54	0.53
	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 344 and name CA)	17.97	0.63	0.62
	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 344 and name CB)	17.69	0.59	0.59
	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 345 and name CA)	15.70	0.77	0.77
	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 345 and name CB)	15.98	0.94	0.94
30	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 346 and name CA)	12.53	0.75	0.75
	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 346 and name CB)	12.72	0.77	0.77
	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 347 and name CA)	10.24	0.76	0.75
	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 347 and name CB)	9.93	0.77	0.77
	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 348 and name CA)	7.53	0.84	0.83
35	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 349 and name CA)	10.52	0.92	0.92
	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 349 and name CB)	11.80	0.94	0.95
	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 350 and name CA)	11.62	0.55	0.55
	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 350 and name CB)	11.99	0.56	0.56
	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 351 and name CA)	8.92	0.33	0.34
40	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 352 and name CA)	9.76	0.46	0.45
	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 352 and name CB)	9.24	0.50	0.50
	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 353 and name CA)	13.41	0.41	0.42
	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 353 and name CB)	14.03	0.39	0.40
	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 354 and name CA)	15.57	0.46	0.47
45	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 354 and name CB)	16.36	0.52	0.53
	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 355 and name CA)	18.13	0.39	0.38
	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 355 and name CB)	18.86	0.39	0.38
	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 356 and name CA)	16.11	0.43	0.43
	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 356 and name CB)	15.29	0.46	0.46
50	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 357 and name CA)	13.99	0.41	0.42
	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 357 and name CB)	12.49	0.42	0.41
	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 358 and name CA)	16.05	0.40	0.40
	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 358 and name CB)	17.20	0.52	0.52
	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 359 and name CA)	14.48	0.30	0.30
55	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 359 and name CB)	15.05	0.31	0.31
	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 360 and name CA)	11.11	0.34	0.33
	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 360 and name CB)	11.34	0.41	0.41
	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 361 and name CA)	10.01	0.28	0.29
	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 361 and name CB)	10.83	0.32	0.31
60	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 362 and name CA)	11.14	0.32	0.33
	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 362 and name CB)	12.57	0.33	0.33
	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 363 and name CA)	9.60	0.45	0.45
	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 363 and name CB)	9.17	0.53	0.54
	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 364 and name CA)	12.40	0.37	0.36
65	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 364 and name CB)	13.28	0.35	0.35
	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 365 and name CA)	13.03	0.25	0.25
	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 365 and name CB)	13.51	0.28	0.27
	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 381 and name CA)	11.16	0.47	0.47
	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 382 and name CA)	11.39	0.42	0.42
70	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 382 and name CB)	12.11	0.52	0.51
	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 383 and name CA)	8.75	0.37	0.37
	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 384 and name CA)	11.98	0.38	0.39
	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 384 and name CB)	12.73	0.41	0.40
	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 385 and name CA)	13.92	0.25	0.26
75	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 386 and name CA)	17.06	0.29	0.28
	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 390 and name CA)	17.75	0.35	0.34
	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 390 and name CB)	18.09	0.42	0.41
	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 391 and name CA)	16.44	0.35	0.34
	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 391 and name CB)	15.07	0.37	0.38
80	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 392 and name CA)	19.48	0.36	0.37
	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 393 and name CA)	17.82	0.46	0.46
	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 394 and name CA)	15.63	0.53	0.53

	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 394 and name CB)	15.69	0.63	0.63
	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 395 and name CA)	18.13	0.61	0.62
	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 396 and name CA)	18.36	0.56	0.56
	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 397 and name CA)	14.64	0.57	0.58
5	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 397 and name CB)	13.66	0.58	0.57
	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 398 and name CA)	14.50	0.58	0.58
	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 398 and name CB)	14.85	0.62	0.62
	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 399 and name CA)	17.73	0.59	0.59
	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 399 and name CB)	18.99	0.56	0.56
	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 400 and name CA)	16.81	0.64	0.64
10	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 400 and name CB)	16.52	0.63	0.63
	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 401 and name CA)	13.74	0.65	0.64
	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 402 and name CA)	15.97	0.58	0.59
	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 402 and name CB)	16.64	0.57	0.56
	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 404 and name CA)	17.38	0.83	0.83
15	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 404 and name CB)	16.34	0.96	0.96
	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 405 and name CA)	15.88	0.57	0.57
	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 405 and name CB)	14.71	0.55	0.55
	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 408 and name CA)	18.29	0.53	0.54
	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 408 and name CB)	14.12	2.27	2.27
20	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 424 and name CA)	13.06	1.82	1.81
	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 425 and name CA)	11.43	1.64	1.65
	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 426 and name CA)	11.52	0.90	0.91
	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 427 and name CA)	13.05	1.14	1.14
	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 428 and name CA)	12.98	0.62	0.62
25	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 429 and name CA)	13.82	0.89	0.89
	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 430 and name CA)	13.18	0.42	0.41
	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 431 and name CA)	8.19	0.71	0.70
	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 433 and name CA)	8.60	0.95	0.94
	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 434 and name CA)	10.15	1.08	1.07
30	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 435 and name CA)	13.72	1.16	1.17
	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 436 and name CA)	15.75	0.95	0.94
	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 437 and name CA)	15.29	0.87	0.88
	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 438 and name CA)	18.64	0.79	0.79
	assign (segid 3A4 and resid 316 and name CA)	(segid 3A4 and resid 439 and name CA)	2.46	0.02	0.03
35	assign (segid 3A4 and resid 316 and name N)	(segid 3A4 and resid 316 and name C)	1.46	0.01	0.01
	assign (segid 3A4 and resid 316 and name N)	(segid 3A4 and resid 316 and name O)	3.36	0.17	0.16
	assign (segid 3A4 and resid 316 and name N)	(segid 3A4 and resid 317 and name C)	5.28	0.16	0.15
	assign (segid 3A4 and resid 316 and name N)	(segid 3A4 and resid 317 and name CA)	4.36	0.12	0.12
40	assign (segid 3A4 and resid 316 and name N)	(segid 3A4 and resid 317 and name N)	2.98	0.18	0.18
	assign (segid 3A4 and resid 316 and name N)	(segid 3A4 and resid 317 and name O)	5.78	0.34	0.34
	assign (segid 3A4 and resid 316 and name N)	(segid 3A4 and resid 318 and name CA)	6.94	0.24	0.24
	assign (segid 3A4 and resid 316 and name N)	(segid 3A4 and resid 318 and name N)	5.87	0.27	0.28
	assign (segid 3A4 and resid 316 and name N)	(segid 3A4 and resid 352 and name CG)	7.28	0.46	0.47
	assign (segid 3A4 and resid 316 and name N)	(segid 3A4 and resid 317 and name C)	2.93	0.21	0.21
45	assign (segid 3A4 and resid 316 and name O)	(segid 3A4 and resid 317 and name CA)	2.79	0.03	0.03
	assign (segid 3A4 and resid 316 and name O)	(segid 3A4 and resid 317 and name N)	2.25	0.02	0.02
	assign (segid 3A4 and resid 316 and name O)	(segid 3A4 and resid 317 and name O)	3.44	0.46	0.47
	assign (segid 3A4 and resid 316 and name O)	(segid 3A4 and resid 318 and name C)	5.38	0.24	0.24
	assign (segid 3A4 and resid 316 and name O)	(segid 3A4 and resid 318 and name CA)	4.15	0.16	0.15
50	assign (segid 3A4 and resid 316 and name O)	(segid 3A4 and resid 318 and name CB)	4.61	0.39	0.38
	assign (segid 3A4 and resid 316 and name O)	(segid 3A4 and resid 318 and name N)	3.29	0.15	0.16
	assign (segid 3A4 and resid 316 and name O)	(segid 3A4 and resid 318 and name O)	6.11	0.33	0.33
	assign (segid 3A4 and resid 316 and name O)	(segid 3A4 and resid 319 and name CA)	7.24	0.29	0.29
	assign (segid 3A4 and resid 316 and name O)	(segid 3A4 and resid 319 and name N)	5.92	0.23	0.24
55	assign (segid 3A4 and resid 316 and name O)	(segid 3A4 and resid 433 and name C)	6.77	0.52	0.53
	assign (segid 3A4 and resid 316 and name O)	(segid 3A4 and resid 433 and name CA)	6.99	0.65	0.65
	assign (segid 3A4 and resid 316 and name O)	(segid 3A4 and resid 433 and name N)	7.22	0.55	0.55
	assign (segid 3A4 and resid 316 and name O)	(segid 3A4 and resid 433 and name O)	6.40	0.47	0.48
60	assign (segid 3A4 and resid 317 and name C)	(segid 3A4 and resid 317 and name O)	1.23	0.00	0.01
	assign (segid 3A4 and resid 317 and name C)	(segid 3A4 and resid 318 and name C)	3.20	0.21	0.21
	assign (segid 3A4 and resid 317 and name C)	(segid 3A4 and resid 318 and name CA)	2.44	0.03	0.02
	assign (segid 3A4 and resid 317 and name C)	(segid 3A4 and resid 318 and name CB)	3.58	0.13	0.14
	assign (segid 3A4 and resid 317 and name C)	(segid 3A4 and resid 318 and name N)	1.35	0.02	0.02
65	assign (segid 3A4 and resid 317 and name C)	(segid 3A4 and resid 318 and name O)	4.16	0.27	0.26
	assign (segid 3A4 and resid 317 and name C)	(segid 3A4 and resid 319 and name C)	4.71	0.52	0.52
	assign (segid 3A4 and resid 317 and name C)	(segid 3A4 and resid 319 and name CA)	4.66	0.33	0.33
	assign (segid 3A4 and resid 317 and name C)	(segid 3A4 and resid 319 and name CB)	5.60	0.24	0.23
	assign (segid 3A4 and resid 317 and name C)	(segid 3A4 and resid 319 and name N)	3.40	0.25	0.25
	assign (segid 3A4 and resid 317 and name C)	(segid 3A4 and resid 319 and name O)	4.88	0.46	0.46
70	assign (segid 3A4 and resid 317 and name C)	(segid 3A4 and resid 347 and name C)	6.80	0.35	0.35
	assign (segid 3A4 and resid 317 and name C)	(segid 3A4 and resid 347 and name CB)	6.84	0.40	0.41
	assign (segid 3A4 and resid 317 and name C)	(segid 3A4 and resid 347 and name O)	7.16	0.36	0.35
	assign (segid 3A4 and resid 317 and name C)	(segid 3A4 and resid 348 and name CA)	5.87	0.64	0.64
	assign (segid 3A4 and resid 317 and name C)	(segid 3A4 and resid 348 and name N)	6.17	0.42	0.42
75	assign (segid 3A4 and resid 317 and name C)	(segid 3A4 and resid 383 and name C)	7.03	0.37	0.37
	assign (segid 3A4 and resid 317 and name C)	(segid 3A4 and resid 383 and name CA)	6.43	0.33	0.32
	assign (segid 3A4 and resid 317 and name C)	(segid 3A4 and resid 383 and name O)	6.50	0.42	0.41
	assign (segid 3A4 and resid 317 and name C)	(segid 3A4 and resid 433 and name C)	6.62	0.37	0.37
	assign (segid 3A4 and resid 317 and name C)	(segid 3A4 and resid 433 and name CA)	6.40	0.47	0.47
80	assign (segid 3A4 and resid 317 and name C)	(segid 3A4 and resid 433 and name N)	6.10	0.41	0.41
	assign (segid 3A4 and resid 317 and name C)	(segid 3A4 and resid 433 and name O)	6.23	0.36	0.37
	assign (segid 3A4 and resid 317 and name C)	(segid HEM and resid 1 and name CHB)	6.32	0.60	0.61

	assign (segid 3A4 and resid 317 and name CA) (segid 3A4 and resid 317 and name C)	1.53	0.01	0.01
	assign (segid 3A4 and resid 317 and name CA) (segid 3A4 and resid 317 and name O)	2.41	0.01	0.01
	assign (segid 3A4 and resid 317 and name CA) (segid 3A4 and resid 318 and name C)	4.61	0.15	0.15
	assign (segid 3A4 and resid 317 and name CA) (segid 3A4 and resid 318 and name CA)	3.82	0.03	0.03
	assign (segid 3A4 and resid 317 and name CA) (segid 3A4 and resid 318 and name CB)	4.73	0.13	0.14
5	assign (segid 3A4 and resid 317 and name CA) (segid 3A4 and resid 318 and name N)	2.47	0.04	0.03
	assign (segid 3A4 and resid 317 and name CA) (segid 3A4 and resid 318 and name O)	5.62	0.21	0.22
	assign (segid 3A4 and resid 317 and name CA) (segid 3A4 and resid 319 and name C)	5.62	0.53	0.53
	assign (segid 3A4 and resid 317 and name CA) (segid 3A4 and resid 319 and name CA)	5.75	0.28	0.28
	assign (segid 3A4 and resid 317 and name CA) (segid 3A4 and resid 319 and name CB)	6.50	0.19	0.18
10	assign (segid 3A4 and resid 317 and name CA) (segid 3A4 and resid 319 and name N)	4.57	0.18	0.19
	assign (segid 3A4 and resid 317 and name CA) (segid 3A4 and resid 319 and name O)	5.52	0.49	0.48
	assign (segid 3A4 and resid 317 and name CA) (segid 3A4 and resid 322 and name CA)	15.45	0.34	0.33
	assign (segid 3A4 and resid 317 and name CA) (segid 3A4 and resid 323 and name CA)	18.39	0.38	0.37
	assign (segid 3A4 and resid 317 and name CA) (segid 3A4 and resid 323 and name CB)	18.19	0.51	0.51
15	assign (segid 3A4 and resid 317 and name CA) (segid 3A4 and resid 343 and name CA)	18.47	0.23	0.23
	assign (segid 3A4 and resid 317 and name CA) (segid 3A4 and resid 343 and name CB)	18.68	0.32	0.31
	assign (segid 3A4 and resid 317 and name CA) (segid 3A4 and resid 344 and name CA)	14.89	0.19	0.19
	assign (segid 3A4 and resid 317 and name CA) (segid 3A4 and resid 344 and name CB)	14.78	0.16	0.15
20	assign (segid 3A4 and resid 317 and name CA) (segid 3A4 and resid 345 and name CA)	12.52	0.35	0.36
	assign (segid 3A4 and resid 317 and name CA) (segid 3A4 and resid 345 and name CB)	12.67	0.63	0.64
	assign (segid 3A4 and resid 317 and name CA) (segid 3A4 and resid 346 and name CA)	9.71	0.24	0.24
	assign (segid 3A4 and resid 317 and name CA) (segid 3A4 and resid 346 and name CB)	10.22	0.40	0.40
	assign (segid 3A4 and resid 317 and name CA) (segid 3A4 and resid 347 and name C)	6.27	0.27	0.26
	assign (segid 3A4 and resid 317 and name CA) (segid 3A4 and resid 347 and name CA)	7.14	0.31	0.30
25	assign (segid 3A4 and resid 317 and name CA) (segid 3A4 and resid 347 and name CB)	6.55	0.46	0.46
	assign (segid 3A4 and resid 317 and name CA) (segid 3A4 and resid 347 and name O)	6.38	0.26	0.26
	assign (segid 3A4 and resid 317 and name CA) (segid 3A4 and resid 348 and name C)	6.56	0.56	0.55
	assign (segid 3A4 and resid 317 and name CA) (segid 3A4 and resid 348 and name CA)	5.38	0.42	0.42
	assign (segid 3A4 and resid 317 and name CA) (segid 3A4 and resid 348 and name N)	5.80	0.29	0.29
30	assign (segid 3A4 and resid 317 and name CA) (segid 3A4 and resid 348 and name O)	6.63	0.69	0.69
	assign (segid 3A4 and resid 317 and name CA) (segid 3A4 and resid 349 and name CA)	8.96	0.56	0.56
	assign (segid 3A4 and resid 317 and name CA) (segid 3A4 and resid 349 and name CB)	10.12	0.51	0.51
	assign (segid 3A4 and resid 317 and name CA) (segid 3A4 and resid 350 and name CA)	9.68	0.28	0.27
35	assign (segid 3A4 and resid 317 and name CA) (segid 3A4 and resid 350 and name CB)	9.69	0.21	0.21
	assign (segid 3A4 and resid 317 and name CA) (segid 3A4 and resid 351 and name CA)	7.72	0.44	0.43
	assign (segid 3A4 and resid 317 and name CA) (segid 3A4 and resid 352 and name CA)	9.58	0.81	0.82
	assign (segid 3A4 and resid 317 and name CA) (segid 3A4 and resid 352 and name CB)	9.25	0.93	0.92
	assign (segid 3A4 and resid 317 and name CA) (segid 3A4 and resid 353 and name CA)	12.76	0.67	0.66
	assign (segid 3A4 and resid 317 and name CA) (segid 3A4 and resid 353 and name CB)	13.02	0.59	0.59
40	assign (segid 3A4 and resid 317 and name CA) (segid 3A4 and resid 354 and name CA)	15.60	0.73	0.73
	assign (segid 3A4 and resid 317 and name CA) (segid 3A4 and resid 354 and name CB)	16.54	0.81	0.80
	assign (segid 3A4 and resid 317 and name CA) (segid 3A4 and resid 355 and name CA)	17.63	0.63	0.64
	assign (segid 3A4 and resid 317 and name CA) (segid 3A4 and resid 355 and name CB)	18.11	0.67	0.68
	assign (segid 3A4 and resid 317 and name CA) (segid 3A4 and resid 356 and name CA)	15.47	0.65	0.64
45	assign (segid 3A4 and resid 317 and name CA) (segid 3A4 and resid 356 and name CB)	14.38	0.68	0.67
	assign (segid 3A4 and resid 317 and name CA) (segid 3A4 and resid 357 and name CA)	14.17	0.56	0.56
	assign (segid 3A4 and resid 317 and name CA) (segid 3A4 and resid 357 and name CB)	12.72	0.57	0.57
	assign (segid 3A4 and resid 317 and name CA) (segid 3A4 and resid 358 and name CA)	16.96	0.82	0.82
	assign (segid 3A4 and resid 317 and name CA) (segid 3A4 and resid 359 and name CA)	16.01	0.72	0.72
50	assign (segid 3A4 and resid 317 and name CA) (segid 3A4 and resid 359 and name CB)	16.79	0.68	0.69
	assign (segid 3A4 and resid 317 and name CA) (segid 3A4 and resid 360 and name CA)	12.31	0.76	0.77
	assign (segid 3A4 and resid 317 and name CA) (segid 3A4 and resid 360 and name CB)	12.16	0.86	0.86
	assign (segid 3A4 and resid 317 and name CA) (segid 3A4 and resid 361 and name CA)	12.08	0.76	0.76
55	assign (segid 3A4 and resid 317 and name CA) (segid 3A4 and resid 361 and name CB)	12.89	0.80	0.81
	assign (segid 3A4 and resid 317 and name CA) (segid 3A4 and resid 362 and name CA)	13.71	0.64	0.64
	assign (segid 3A4 and resid 317 and name CA) (segid 3A4 and resid 362 and name CB)	15.04	0.63	0.64
	assign (segid 3A4 and resid 317 and name CA) (segid 3A4 and resid 363 and name CA)	12.45	0.48	0.47
	assign (segid 3A4 and resid 317 and name CA) (segid 3A4 and resid 363 and name CB)	12.29	0.49	0.49
60	assign (segid 3A4 and resid 317 and name CA) (segid 3A4 and resid 364 and name CA)	14.77	0.32	0.31
	assign (segid 3A4 and resid 317 and name CA) (segid 3A4 and resid 364 and name CB)	15.51	0.36	0.36
	assign (segid 3A4 and resid 317 and name CA) (segid 3A4 and resid 365 and name CA)	15.03	0.21	0.20
	assign (segid 3A4 and resid 317 and name CA) (segid 3A4 and resid 365 and name CB)	15.63	0.17	0.17
	assign (segid 3A4 and resid 317 and name CA) (segid 3A4 and resid 381 and name CA)	9.38	0.53	0.54
65	assign (segid 3A4 and resid 317 and name CA) (segid 3A4 and resid 382 and name CA)	8.54	0.42	0.41
	assign (segid 3A4 and resid 317 and name CA) (segid 3A4 and resid 382 and name CB)	9.13	0.43	0.43
	assign (segid 3A4 and resid 317 and name CA) (segid 3A4 and resid 383 and name C)	6.57	0.48	0.48
	assign (segid 3A4 and resid 317 and name CA) (segid 3A4 and resid 383 and name N)	5.70	0.45	0.45
	assign (segid 3A4 and resid 317 and name CA) (segid 3A4 and resid 383 and name O)	6.66	0.43	0.44
70	assign (segid 3A4 and resid 317 and name CA) (segid 3A4 and resid 383 and name O)	6.29	0.51	0.50
	assign (segid 3A4 and resid 317 and name CA) (segid 3A4 and resid 384 and name CA)	8.89	0.49	0.49
	assign (segid 3A4 and resid 317 and name CA) (segid 3A4 and resid 384 and name CB)	9.89	0.54	0.53
	assign (segid 3A4 and resid 317 and name CA) (segid 3A4 and resid 385 and name CA)	10.44	0.29	0.29
75	assign (segid 3A4 and resid 317 and name CA) (segid 3A4 and resid 386 and name CA)	13.73	0.31	0.31
	assign (segid 3A4 and resid 317 and name CA) (segid 3A4 and resid 387 and name CA)	17.20	0.13	0.12
	assign (segid 3A4 and resid 317 and name CA) (segid 3A4 and resid 389 and name CA)	16.84	0.44	0.44
	assign (segid 3A4 and resid 317 and name CA) (segid 3A4 and resid 389 and name CB)	16.62	0.49	0.50
	assign (segid 3A4 and resid 317 and name CA) (segid 3A4 and resid 390 and name CA)	14.41	0.45	0.45
	assign (segid 3A4 and resid 317 and name CA) (segid 3A4 and resid 390 and name CB)	14.85	0.51	0.51
	assign (segid 3A4 and resid 317 and name CA) (segid 3A4 and resid 391 and name CA)	13.36	0.49	0.49
80	assign (segid 3A4 and resid 317 and name CA) (segid 3A4 and resid 391 and name CB)	12.11	0.55	0.55
	assign (segid 3A4 and resid 317 and name CA) (segid 3A4 and resid 392 and name CA)	16.67	0.48	0.48
	assign (segid 3A4 and resid 317 and name CA) (segid 3A4 and resid 392 and name CB)	17.71	0.44	0.45

	assign (segid 3A4 and resid 317 and name CA)	(segid 3A4 and resid 393 and name CA)	15.51	0.62	0.62
	assign (segid 3A4 and resid 317 and name CA)	(segid 3A4 and resid 394 and name CA)	13.48	0.60	0.60
	assign (segid 3A4 and resid 317 and name CA)	(segid 3A4 and resid 394 and name CB)	13.40	0.68	0.67
	assign (segid 3A4 and resid 317 and name CA)	(segid 3A4 and resid 395 and name CA)	16.49	0.65	0.65
	assign (segid 3A4 and resid 317 and name CA)	(segid 3A4 and resid 396 and name CA)	16.99	0.69	0.68
5	assign (segid 3A4 and resid 317 and name CA)	(segid 3A4 and resid 396 and name CB)	17.48	0.82	0.83
	assign (segid 3A4 and resid 317 and name CA)	(segid 3A4 and resid 397 and name CA)	13.46	0.67	0.66
	assign (segid 3A4 and resid 317 and name CA)	(segid 3A4 and resid 397 and name CB)	12.22	0.69	0.69
	assign (segid 3A4 and resid 317 and name CA)	(segid 3A4 and resid 398 and name CA)	13.79	0.55	0.55
	assign (segid 3A4 and resid 317 and name CA)	(segid 3A4 and resid 398 and name CB)	14.00	0.62	0.63
10	assign (segid 3A4 and resid 317 and name CA)	(segid 3A4 and resid 399 and name CA)	17.31	0.48	0.48
	assign (segid 3A4 and resid 317 and name CA)	(segid 3A4 and resid 399 and name CB)	18.39	0.51	0.51
	assign (segid 3A4 and resid 317 and name CA)	(segid 3A4 and resid 400 and name CA)	16.69	0.58	0.58
	assign (segid 3A4 and resid 317 and name CA)	(segid 3A4 and resid 400 and name CB)	16.23	0.62	0.62
	assign (segid 3A4 and resid 317 and name CA)	(segid 3A4 and resid 401 and name CA)	14.17	0.51	0.52
15	assign (segid 3A4 and resid 317 and name CA)	(segid 3A4 and resid 402 and name CA)	16.64	0.46	0.47
	assign (segid 3A4 and resid 317 and name CA)	(segid 3A4 and resid 402 and name CB)	17.09	0.46	0.47
	assign (segid 3A4 and resid 317 and name CA)	(segid 3A4 and resid 404 and name CA)	18.50	0.63	0.63
	assign (segid 3A4 and resid 317 and name CA)	(segid 3A4 and resid 404 and name CB)	17.39	0.68	0.68
	assign (segid 3A4 and resid 317 and name CA)	(segid 3A4 and resid 405 and name CA)	17.55	0.48	0.48
20	assign (segid 3A4 and resid 317 and name CA)	(segid 3A4 and resid 405 and name CB)	16.39	0.44	0.44
	assign (segid 3A4 and resid 317 and name CA)	(segid 3A4 and resid 405 and name CB)	15.45	1.70	1.69
	assign (segid 3A4 and resid 317 and name CA)	(segid 3A4 and resid 425 and name CA)	13.25	1.83	1.82
	assign (segid 3A4 and resid 317 and name CA)	(segid 3A4 and resid 426 and name CA)	12.44	0.56	0.57
	assign (segid 3A4 and resid 317 and name CA)	(segid 3A4 and resid 427 and name CA)	13.20	1.22	1.22
25	assign (segid 3A4 and resid 317 and name CA)	(segid 3A4 and resid 428 and name CA)	12.44	0.57	0.57
	assign (segid 3A4 and resid 317 and name CA)	(segid 3A4 and resid 429 and name CA)	12.37	1.03	1.03
	assign (segid 3A4 and resid 317 and name CA)	(segid 3A4 and resid 430 and name CA)	11.05	0.56	0.56
	assign (segid 3A4 and resid 317 and name CA)	(segid 3A4 and resid 431 and name CA)	7.76	0.51	0.52
	assign (segid 3A4 and resid 317 and name CA)	(segid 3A4 and resid 433 and name CA)	9.29	0.81	0.82
30	assign (segid 3A4 and resid 317 and name CA)	(segid 3A4 and resid 434 and name CA)	11.90	0.76	0.76
	assign (segid 3A4 and resid 317 and name CA)	(segid 3A4 and resid 435 and name CA)	15.23	0.80	0.80
	assign (segid 3A4 and resid 317 and name CA)	(segid 3A4 and resid 436 and name CA)	17.76	0.66	0.66
	assign (segid 3A4 and resid 317 and name CA)	(segid 3A4 and resid 437 and name CA)	17.84	0.73	0.72
	assign (segid 3A4 and resid 317 and name CA)	(segid 3A4 and resid 438 and name CA)	2.45	0.03	0.02
35	assign (segid 3A4 and resid 317 and name N)	(segid 3A4 and resid 317 and name CA)	1.47	0.01	0.02
	assign (segid 3A4 and resid 317 and name N)	(segid 3A4 and resid 317 and name CA)	3.08	0.20	0.19
	assign (segid 3A4 and resid 317 and name N)	(segid 3A4 and resid 318 and name C)	5.55	0.22	0.23
	assign (segid 3A4 and resid 317 and name N)	(segid 3A4 and resid 318 and name CA)	4.52	0.15	0.16
40	assign (segid 3A4 and resid 317 and name N)	(segid 3A4 and resid 318 and name CB)	5.29	0.23	0.23
	assign (segid 3A4 and resid 317 and name N)	(segid 3A4 and resid 318 and name N)	3.29	0.22	0.22
	assign (segid 3A4 and resid 317 and name N)	(segid 3A4 and resid 318 and name O)	6.46	0.27	0.28
	assign (segid 3A4 and resid 317 and name N)	(segid 3A4 and resid 319 and name CA)	6.98	0.34	0.35
	assign (segid 3A4 and resid 317 and name N)	(segid 3A4 and resid 319 and name N)	5.75	0.26	0.26
45	assign (segid 3A4 and resid 317 and name N)	(segid 3A4 and resid 319 and name O)	6.82	0.54	0.55
	assign (segid 3A4 and resid 317 and name N)	(segid 3A4 and resid 347 and name O)	7.02	0.42	0.42
	assign (segid 3A4 and resid 317 and name N)	(segid 3A4 and resid 348 and name CA)	5.85	0.52	0.52
	assign (segid 3A4 and resid 317 and name N)	(segid 3A4 and resid 348 and name N)	6.52	0.53	0.53
	assign (segid 3A4 and resid 317 and name N)	(segid 3A4 and resid 348 and name O)	6.70	0.67	0.67
	assign (segid 3A4 and resid 317 and name N)	(segid 3A4 and resid 383 and name CA)	6.65	0.35	0.36
50	assign (segid 3A4 and resid 317 and name N)	(segid 3A4 and resid 318 and name C)	3.15	0.32	0.33
	assign (segid 3A4 and resid 317 and name O)	(segid 3A4 and resid 318 and name CA)	2.73	0.06	0.06
	assign (segid 3A4 and resid 317 and name O)	(segid 3A4 and resid 318 and name CB)	4.08	0.22	0.22
	assign (segid 3A4 and resid 317 and name O)	(segid 3A4 and resid 318 and name N)	2.24	0.02	0.03
	assign (segid 3A4 and resid 317 and name O)	(segid 3A4 and resid 318 and name O)	3.84	0.43	0.43
55	assign (segid 3A4 and resid 317 and name O)	(segid 3A4 and resid 319 and name C)	4.40	0.75	0.76
	assign (segid 3A4 and resid 317 and name O)	(segid 3A4 and resid 319 and name CA)	4.55	0.56	0.55
	assign (segid 3A4 and resid 317 and name O)	(segid 3A4 and resid 319 and name CB)	5.72	0.45	0.45
	assign (segid 3A4 and resid 317 and name O)	(segid 3A4 and resid 319 and name N)	3.50	0.41	0.40
	assign (segid 3A4 and resid 317 and name O)	(segid 3A4 and resid 319 and name O)	4.71	0.63	0.64
60	assign (segid 3A4 and resid 317 and name O)	(segid 3A4 and resid 347 and name C)	6.74	0.35	0.35
	assign (segid 3A4 and resid 317 and name O)	(segid 3A4 and resid 347 and name CB)	6.92	0.57	0.58
	assign (segid 3A4 and resid 317 and name O)	(segid 3A4 and resid 347 and name O)	7.23	0.32	0.32
	assign (segid 3A4 and resid 317 and name O)	(segid 3A4 and resid 348 and name C)	6.91	0.72	0.71
	assign (segid 3A4 and resid 317 and name O)	(segid 3A4 and resid 348 and name CA)	5.59	0.54	0.55
65	assign (segid 3A4 and resid 317 and name O)	(segid 3A4 and resid 348 and name N)	5.93	0.39	0.39
	assign (segid 3A4 and resid 317 and name O)	(segid 3A4 and resid 433 and name C)	6.19	0.42	0.42
	assign (segid 3A4 and resid 317 and name O)	(segid 3A4 and resid 433 and name CA)	5.77	0.56	0.56
	assign (segid 3A4 and resid 317 and name O)	(segid 3A4 and resid 433 and name N)	5.50	0.55	0.55
	assign (segid 3A4 and resid 317 and name O)	(segid 3A4 and resid 433 and name O)	6.00	0.41	0.40
70	assign (segid 3A4 and resid 318 and name C)	(segid 3A4 and resid 318 and name CB)	2.53	0.03	0.03
	assign (segid 3A4 and resid 318 and name C)	(segid 3A4 and resid 318 and name O)	1.22	0.00	0.01
	assign (segid 3A4 and resid 318 and name C)	(segid 3A4 and resid 319 and name C)	3.32	0.14	0.13
	assign (segid 3A4 and resid 318 and name C)	(segid 3A4 and resid 319 and name CA)	2.44	0.02	0.02
	assign (segid 3A4 and resid 318 and name C)	(segid 3A4 and resid 319 and name CB)	3.55	0.08	0.08
75	assign (segid 3A4 and resid 318 and name C)	(segid 3A4 and resid 319 and name N)	1.33	0.00	0.01
	assign (segid 3A4 and resid 318 and name C)	(segid 3A4 and resid 319 and name O)	4.10	0.22	0.23
	assign (segid 3A4 and resid 318 and name C)	(segid 3A4 and resid 383 and name C)	7.62	0.07	0.08
	assign (segid 3A4 and resid 318 and name C)	(segid 3A4 and resid 383 and name CA)	7.63	0.16	0.15
	assign (segid 3A4 and resid 318 and name C)	(segid 3A4 and resid 383 and name O)	6.67	0.10	0.10
80	assign (segid 3A4 and resid 318 and name C)	(segid 3A4 and resid 431 and name C)	5.80	0.75	0.74
	assign (segid 3A4 and resid 318 and name C)	(segid 3A4 and resid 431 and name O)	5.30	0.98	0.99
	assign (segid 3A4 and resid 318 and name C)	(segid 3A4 and resid 433 and name C)	5.37	0.27	0.26

	assign (segid 3A4 and resid 318 and name C) (segid 3A4 and resid 433 and name CA)	5.05	0.27	0.27
	assign (segid 3A4 and resid 318 and name C) (segid 3A4 and resid 433 and name N)	4.17	0.33	0.33
	assign (segid 3A4 and resid 318 and name C) (segid 3A4 and resid 433 and name O)	4.86	0.27	0.27
	assign (segid 3A4 and resid 318 and name C) (segid 3A4 and resid 434 and name CA)	7.28	0.61	0.60
5	assign (segid 3A4 and resid 318 and name C) (segid 3A4 and resid 434 and name N)	6.52	0.45	0.45
	assign (segid 3A4 and resid 318 and name C) (segid HEM and resid 1 and name C1B)	7.25	0.43	0.42
	assign (segid 3A4 and resid 318 and name C) (segid HEM and resid 1 and name C2B)	6.76	0.48	0.47
	assign (segid 3A4 and resid 318 and name C) (segid HEM and resid 1 and name CHB)	7.00	0.32	0.31
	assign (segid 3A4 and resid 318 and name C) (segid HEM and resid 1 and name CMA)	7.22	0.12	0.13
	assign (segid 3A4 and resid 318 and name C) (segid HEM and resid 1 and name CMB)	5.79	0.44	0.44
10	assign (segid 3A4 and resid 318 and name C) (segid 3A4 and resid 318 and name C)	1.52	0.01	0.02
	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 318 and name CB)	1.54	0.03	0.02
	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 318 and name O)	2.39	0.01	0.01
	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 319 and name C)	4.56	0.11	0.10
	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 319 and name CB)	3.82	0.03	0.03
15	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 319 and name N)	4.76	0.06	0.07
	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 319 and name O)	2.45	0.03	0.03
	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 319 and name CB)	5.14	0.26	0.26
	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 322 and name CA)	14.76	0.58	0.59
	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 322 and name CB)	18.02	0.65	0.65
20	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 323 and name CA)	18.11	0.71	0.72
	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 323 and name CB)	18.55	0.58	0.57
	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 343 and name CA)	18.96	0.50	0.50
	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 343 and name CB)	14.93	0.60	0.59
	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 344 and name CA)	14.67	0.64	0.64
25	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 344 and name CB)	13.31	0.48	0.48
	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 345 and name CA)	13.50	0.46	0.47
	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 345 and name CB)	10.86	0.84	0.84
	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 346 and name CA)	11.46	1.07	1.07
	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 346 and name CB)	8.98	0.62	0.61
30	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 347 and name CA)	8.10	0.54	0.53
	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 347 and name CB)	7.79	0.98	0.99
	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 348 and name CA)	11.52	1.05	1.05
	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 349 and name CA)	12.40	1.06	1.05
	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 349 and name CB)	12.66	0.63	0.62
35	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 350 and name CA)	12.51	0.49	0.50
	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 350 and name CB)	11.25	0.54	0.53
	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 351 and name CA)	13.02	0.97	0.97
	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 352 and name CA)	12.51	1.12	1.11
	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 352 and name CB)	16.13	0.92	0.92
40	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 353 and name CA)	16.33	0.90	0.90
	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 353 and name CB)	17.89	0.90	0.91
	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 356 and name CA)	17.87	0.65	0.65
	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 357 and name CA)	16.42	0.64	0.64
	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 357 and name CB)	15.81	0.75	0.75
45	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 360 and name CA)	15.67	0.89	0.88
	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 360 and name CB)	15.15	0.72	0.71
	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 361 and name CA)	15.81	0.81	0.80
	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 361 and name CB)	16.72	0.53	0.54
	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 362 and name CA)	18.13	0.54	0.53
50	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 362 and name CB)	15.21	0.44	0.44
	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 363 and name CA)	14.77	0.43	0.43
	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 363 and name CB)	17.70	0.36	0.36
	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 364 and name CA)	18.60	0.36	0.36
	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 364 and name CB)	17.69	0.46	0.47
55	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 365 and name CA)	18.06	0.47	0.47
	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 365 and name CB)	12.43	0.48	0.47
	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 382 and name CA)	10.86	0.26	0.26
	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 382 and name CB)	11.40	0.29	0.30
	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 382 and name C)	7.68	0.06	0.05
60	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 383 and name CA)	7.51	0.14	0.14
	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 383 and name O)	6.84	0.05	0.06
	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 384 and name CA)	9.50	0.07	0.07
	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 384 and name CB)	10.52	0.12	0.12
65	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 385 and name CA)	11.23	0.18	0.18
	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 386 and name CA)	14.89	0.24	0.24
	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 387 and name CA)	18.04	0.39	0.40
	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 388 and name CA)	19.55	0.16	0.16
	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 389 and name CA)	16.57	0.24	0.24
	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 389 and name CB)	16.24	0.42	0.42
70	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 390 and name CA)	14.57	0.17	0.17
	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 390 and name CB)	15.31	0.29	0.30
	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 391 and name CA)	12.85	0.26	0.26
	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 391 and name CB)	11.61	0.28	0.28
	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 392 and name CA)	15.89	0.28	0.29
75	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 392 and name CB)	16.70	0.35	0.34
	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 393 and name CA)	14.45	0.38	0.37
	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 394 and name CA)	13.28	0.29	0.29
	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 394 and name CB)	13.54	0.24	0.24
	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 395 and name CA)	16.41	0.38	0.37
80	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 396 and name CA)	16.15	0.48	0.48
	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 396 and name CB)	16.37	0.60	0.60
	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 397 and name CA)	12.60	0.47	0.47

	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 397 and name CB)	11.37	0.46	0.47
	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 398 and name CA)	13.88	0.42	0.42
	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 398 and name CB)	14.41	0.46	0.47
	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 399 and name CA)	17.07	0.40	0.40
5	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 399 and name CB)	18.03	0.45	0.44
	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 400 and name CA)	15.79	0.46	0.46
	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 400 and name CB)	15.03	0.52	0.53
	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 401 and name CA)	13.76	0.45	0.45
	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 402 and name CA)	16.85	0.45	0.45
10	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 402 and name CB)	17.47	0.44	0.45
	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 404 and name CA)	17.78	0.44	0.43
	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 404 and name CB)	16.49	0.43	0.42
	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 405 and name CA)	17.47	0.62	0.63
	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 405 and name CB)	16.55	0.69	0.68
15	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 424 and name CA)	16.31	1.88	1.87
	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 425 and name CA)	14.40	1.08	1.08
	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 426 and name CA)	11.81	1.54	1.54
	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 427 and name CA)	10.40	0.27	0.27
	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 428 and name CA)	10.97	1.05	1.04
20	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 429 and name CA)	10.03	0.95	0.95
	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 430 and name CA)	10.06	1.06	1.06
	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 431 and name CA)	8.36	0.51	0.51
	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 433 and name C)	5.07	0.29	0.30
	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 433 and name CA)	5.05	0.16	0.15
25	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 433 and name N)	4.52	0.16	0.17
	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 433 and name O)	4.45	0.36	0.36
	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 434 and name CA)	6.70	0.73	0.74
	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 434 and name N)	6.14	0.50	0.51
30	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 435 and name CA)	9.86	0.60	0.61
	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 436 and name CA)	12.82	0.79	0.80
	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 437 and name CA)	15.62	0.67	0.66
	assign (segid 3A4 and resid 318 and name CA) (segid 3A4 and resid 438 and name CA)	16.27	0.76	0.76
	assign (segid 3A4 and resid 318 and name CA) (segid HEM and resid 1 and name C2B)	6.80	0.40	0.39
	assign (segid 3A4 and resid 318 and name CA) (segid HEM and resid 1 and name CBB)	7.28	0.45	0.45
35	assign (segid 3A4 and resid 318 and name CA) (segid HEM and resid 1 and name CHB)	7.49	0.25	0.24
	assign (segid 3A4 and resid 318 and name CA) (segid HEM and resid 1 and name CMB)	5.66	0.36	0.37
	assign (segid 3A4 and resid 318 and name CB) (segid 3A4 and resid 319 and name C)	5.67	0.12	0.12
	assign (segid 3A4 and resid 318 and name CB) (segid 3A4 and resid 319 and name CA)	4.65	0.09	0.09
	assign (segid 3A4 and resid 318 and name CB) (segid 3A4 and resid 319 and name CB)	5.28	0.19	0.18
40	assign (segid 3A4 and resid 318 and name CB) (segid 3A4 and resid 319 and name N)	3.35	0.12	0.12
	assign (segid 3A4 and resid 318 and name CB) (segid 3A4 and resid 319 and name O)	6.24	0.11	0.11
	assign (segid 3A4 and resid 318 and name CB) (segid 3A4 and resid 322 and name CA)	15.64	0.68	0.69
	assign (segid 3A4 and resid 318 and name CB) (segid 3A4 and resid 344 and name CA)	16.10	0.64	0.63
	assign (segid 3A4 and resid 318 and name CB) (segid 3A4 and resid 344 and name CB)	15.88	0.69	0.68
45	assign (segid 3A4 and resid 318 and name CB) (segid 3A4 and resid 345 and name CA)	14.49	0.49	0.50
	assign (segid 3A4 and resid 318 and name CB) (segid 3A4 and resid 345 and name CB)	14.60	0.56	0.55
	assign (segid 3A4 and resid 318 and name CB) (segid 3A4 and resid 346 and name CA)	12.21	0.78	0.77
	assign (segid 3A4 and resid 318 and name CB) (segid 3A4 and resid 346 and name CB)	12.86	1.00	0.99
	assign (segid 3A4 and resid 318 and name CB) (segid 3A4 and resid 347 and name CA)	10.16	0.58	0.58
50	assign (segid 3A4 and resid 318 and name CB) (segid 3A4 and resid 347 and name CB)	9.17	0.55	0.55
	assign (segid 3A4 and resid 318 and name CB) (segid 3A4 and resid 348 and name CA)	9.14	0.92	0.92
	assign (segid 3A4 and resid 318 and name CB) (segid 3A4 and resid 349 and name CA)	12.87	0.99	1.00
	assign (segid 3A4 and resid 318 and name CB) (segid 3A4 and resid 349 and name CB)	13.78	0.99	0.99
	assign (segid 3A4 and resid 318 and name CB) (segid 3A4 and resid 350 and name CA)	13.81	0.61	0.62
55	assign (segid 3A4 and resid 318 and name CB) (segid 3A4 and resid 350 and name CB)	13.62	0.50	0.49
	assign (segid 3A4 and resid 318 and name CB) (segid 3A4 and resid 351 and name CA)	12.21	0.65	0.65
	assign (segid 3A4 and resid 318 and name CB) (segid 3A4 and resid 352 and name CA)	14.10	1.00	1.01
	assign (segid 3A4 and resid 318 and name CB) (segid 3A4 and resid 352 and name CB)	13.65	1.14	1.14
	assign (segid 3A4 and resid 318 and name CB) (segid 3A4 and resid 353 and name CA)	17.25	0.93	0.94
60	assign (segid 3A4 and resid 318 and name CB) (segid 3A4 and resid 353 and name CB)	17.45	0.89	0.90
	assign (segid 3A4 and resid 318 and name CB) (segid 3A4 and resid 357 and name CB)	17.18	0.69	0.70
	assign (segid 3A4 and resid 318 and name CB) (segid 3A4 and resid 360 and name CA)	16.64	0.76	0.77
	assign (segid 3A4 and resid 318 and name CB) (segid 3A4 and resid 360 and name CB)	16.60	0.91	0.90
	assign (segid 3A4 and resid 318 and name CB) (segid 3A4 and resid 361 and name CA)	15.94	0.75	0.76
65	assign (segid 3A4 and resid 318 and name CB) (segid 3A4 and resid 361 and name CB)	16.66	0.87	0.87
	assign (segid 3A4 and resid 318 and name CB) (segid 3A4 and resid 362 and name CA)	17.24	0.53	0.54
	assign (segid 3A4 and resid 318 and name CB) (segid 3A4 and resid 362 and name CB)	18.64	0.53	0.53
	assign (segid 3A4 and resid 318 and name CB) (segid 3A4 and resid 363 and name CA)	15.45	0.41	0.40
	assign (segid 3A4 and resid 318 and name CB) (segid 3A4 and resid 363 and name CB)	14.91	0.40	0.41
70	assign (segid 3A4 and resid 318 and name CB) (segid 3A4 and resid 364 and name CA)	17.82	0.35	0.35
	assign (segid 3A4 and resid 318 and name CB) (segid 3A4 and resid 364 and name CB)	18.81	0.34	0.35
	assign (segid 3A4 and resid 318 and name CB) (segid 3A4 and resid 365 and name CA)	17.56	0.48	0.47
	assign (segid 3A4 and resid 318 and name CB) (segid 3A4 and resid 365 and name CB)	17.81	0.49	0.49
	assign (segid 3A4 and resid 318 and name CB) (segid 3A4 and resid 381 and name CA)	12.92	0.50	0.49
75	assign (segid 3A4 and resid 318 and name CB) (segid 3A4 and resid 382 and name CA)	11.44	0.38	0.37
	assign (segid 3A4 and resid 318 and name CB) (segid 3A4 and resid 382 and name CB)	12.12	0.40	0.40
	assign (segid 3A4 and resid 318 and name CB) (segid 3A4 and resid 383 and name CA)	7.85	0.36	0.37
	assign (segid 3A4 and resid 318 and name CB) (segid 3A4 and resid 383 and name O)	7.00	0.35	0.34
	assign (segid 3A4 and resid 318 and name CB) (segid 3A4 and resid 384 and name CA)	9.48	0.35	0.35
80	assign (segid 3A4 and resid 318 and name CB) (segid 3A4 and resid 384 and name CB)	10.35	0.32	0.31
	assign (segid 3A4 and resid 318 and name CB) (segid 3A4 and resid 385 and name CA)	11.62	0.42	0.41
	assign (segid 3A4 and resid 318 and name CB) (segid 3A4 and resid 386 and name CA)	15.30	0.42	0.42
	assign (segid 3A4 and resid 318 and name CB) (segid 3A4 and resid 387 and name CA)	18.39	0.65	0.65

	assign (segid 3A4 and resid 318 and name CB)	(segid 3A4 and resid 389 and name CA)	16.69	0.45	0.45
	assign (segid 3A4 and resid 318 and name CB)	(segid 3A4 and resid 389 and name CB)	16.45	0.57	0.58
	assign (segid 3A4 and resid 318 and name CB)	(segid 3A4 and resid 390 and name CA)	14.59	0.41	0.41
	assign (segid 3A4 and resid 318 and name CB)	(segid 3A4 and resid 390 and name CB)	15.32	0.48	0.49
	assign (segid 3A4 and resid 318 and name CB)	(segid 3A4 and resid 391 and name CA)	12.53	0.49	0.48
5	assign (segid 3A4 and resid 318 and name CB)	(segid 3A4 and resid 391 and name CB)	11.22	0.43	0.44
	assign (segid 3A4 and resid 318 and name CB)	(segid 3A4 and resid 392 and name CA)	15.34	0.53	0.52
	assign (segid 3A4 and resid 318 and name CB)	(segid 3A4 and resid 392 and name CB)	16.13	0.60	0.61
	assign (segid 3A4 and resid 318 and name CB)	(segid 3A4 and resid 393 and name CA)	13.60	0.49	0.49
	assign (segid 3A4 and resid 318 and name CB)	(segid 3A4 and resid 394 and name CA)	12.54	0.38	0.39
10	assign (segid 3A4 and resid 318 and name CB)	(segid 3A4 and resid 394 and name CB)	12.94	0.27	0.27
	assign (segid 3A4 and resid 318 and name CB)	(segid 3A4 and resid 395 and name CA)	15.52	0.43	0.42
	assign (segid 3A4 and resid 318 and name CB)	(segid 3A4 and resid 395 and name CB)	15.03	0.51	0.52
	assign (segid 3A4 and resid 318 and name CB)	(segid 3A4 and resid 396 and name CA)	15.24	0.60	0.60
	assign (segid 3A4 and resid 318 and name CB)	(segid 3A4 and resid 396 and name CB)	11.44	0.51	0.51
15	assign (segid 3A4 and resid 318 and name CB)	(segid 3A4 and resid 397 and name CB)	10.28	0.51	0.50
	assign (segid 3A4 and resid 318 and name CB)	(segid 3A4 and resid 397 and name CB)	12.86	0.48	0.47
	assign (segid 3A4 and resid 318 and name CB)	(segid 3A4 and resid 398 and name CA)	13.50	0.49	0.49
	assign (segid 3A4 and resid 318 and name CB)	(segid 3A4 and resid 398 and name CB)	15.91	0.47	0.47
20	assign (segid 3A4 and resid 318 and name CB)	(segid 3A4 and resid 399 and name CA)	16.86	0.52	0.51
	assign (segid 3A4 and resid 318 and name CB)	(segid 3A4 and resid 399 and name CB)	14.47	0.49	0.49
	assign (segid 3A4 and resid 318 and name CB)	(segid 3A4 and resid 400 and name CA)	13.67	0.54	0.55
	assign (segid 3A4 and resid 318 and name CB)	(segid 3A4 and resid 400 and name CB)	12.52	0.48	0.47
	assign (segid 3A4 and resid 318 and name CB)	(segid 3A4 and resid 401 and name CA)	15.73	0.48	0.49
	assign (segid 3A4 and resid 318 and name CB)	(segid 3A4 and resid 401 and name CB)	16.40	0.48	0.49
25	assign (segid 3A4 and resid 318 and name CB)	(segid 3A4 and resid 402 and name CA)	18.02	0.46	0.45
	assign (segid 3A4 and resid 318 and name CB)	(segid 3A4 and resid 402 and name CB)	18.33	0.50	0.51
	assign (segid 3A4 and resid 318 and name CB)	(segid 3A4 and resid 403 and name CA)	16.46	0.43	0.44
	assign (segid 3A4 and resid 318 and name CB)	(segid 3A4 and resid 403 and name CB)	15.14	0.42	0.42
30	assign (segid 3A4 and resid 318 and name CB)	(segid 3A4 and resid 404 and name CA)	16.33	0.61	0.62
	assign (segid 3A4 and resid 318 and name CB)	(segid 3A4 and resid 404 and name CB)	15.47	0.68	0.68
	assign (segid 3A4 and resid 318 and name CB)	(segid 3A4 and resid 405 and name CA)	18.63	0.52	0.53
	assign (segid 3A4 and resid 318 and name CB)	(segid 3A4 and resid 405 and name CB)	16.23	1.58	1.58
	assign (segid 3A4 and resid 318 and name CB)	(segid 3A4 and resid 408 and name CA)	14.43	0.69	0.69
	assign (segid 3A4 and resid 318 and name CB)	(segid 3A4 and resid 424 and name CA)	11.99	1.18	1.18
35	assign (segid 3A4 and resid 318 and name CB)	(segid 3A4 and resid 425 and name CA)	10.63	0.39	0.39
	assign (segid 3A4 and resid 318 and name CB)	(segid 3A4 and resid 426 and name CA)	11.40	1.06	1.06
	assign (segid 3A4 and resid 318 and name CB)	(segid 3A4 and resid 427 and name CA)	10.62	1.06	1.06
	assign (segid 3A4 and resid 318 and name CB)	(segid 3A4 and resid 429 and name CA)	10.79	1.11	1.11
40	assign (segid 3A4 and resid 318 and name CB)	(segid 3A4 and resid 430 and name CA)	8.97	0.50	0.50
	assign (segid 3A4 and resid 318 and name CB)	(segid 3A4 and resid 431 and name CA)	5.14	0.38	0.38
	assign (segid 3A4 and resid 318 and name CB)	(segid 3A4 and resid 433 and name C)	5.46	0.34	0.33
	assign (segid 3A4 and resid 318 and name CB)	(segid 3A4 and resid 433 and name N)	4.97	0.32	0.32
	assign (segid 3A4 and resid 318 and name CB)	(segid 3A4 and resid 433 and name O)	4.25	0.39	0.40
45	assign (segid 3A4 and resid 318 and name CB)	(segid 3A4 and resid 434 and name CA)	6.47	0.68	0.68
	assign (segid 3A4 and resid 318 and name CB)	(segid 3A4 and resid 434 and name N)	6.17	0.52	0.51
	assign (segid 3A4 and resid 318 and name CB)	(segid 3A4 and resid 435 and name CA)	9.49	0.53	0.53
	assign (segid 3A4 and resid 318 and name CB)	(segid 3A4 and resid 436 and name CA)	12.39	0.84	0.83
	assign (segid 3A4 and resid 318 and name CB)	(segid 3A4 and resid 437 and name CA)	15.05	0.71	0.71
50	assign (segid 3A4 and resid 318 and name CB)	(segid 3A4 and resid 438 and name CA)	15.63	0.91	0.90
	assign (segid 3A4 and resid 318 and name CB)	(segid HEM and resid 1 and name C2B)	6.09	0.43	0.44
	assign (segid 3A4 and resid 318 and name CB)	(segid HEM and resid 1 and name C3B)	6.67	0.46	0.46
	assign (segid 3A4 and resid 318 and name CB)	(segid HEM and resid 1 and name CAB)	6.65	0.48	0.48
	assign (segid 3A4 and resid 318 and name CB)	(segid HEM and resid 1 and name CBB)	6.16	0.44	0.44
	assign (segid 3A4 and resid 318 and name CB)	(segid HEM and resid 1 and name CMB)	5.09	0.39	0.39
55	assign (segid 3A4 and resid 318 and name CB)	(segid 3A4 and resid 318 and name C)	2.52	0.03	0.03
	assign (segid 3A4 and resid 318 and name N)	(segid 3A4 and resid 318 and name CA)	1.45	0.01	0.01
	assign (segid 3A4 and resid 318 and name N)	(segid 3A4 and resid 318 and name CB)	2.39	0.03	0.03
	assign (segid 3A4 and resid 318 and name N)	(segid 3A4 and resid 318 and name O)	3.59	0.05	0.05
60	assign (segid 3A4 and resid 318 and name N)	(segid 3A4 and resid 319 and name C)	4.73	0.15	0.15
	assign (segid 3A4 and resid 318 and name N)	(segid 3A4 and resid 319 and name CA)	4.28	0.04	0.04
	assign (segid 3A4 and resid 318 and name N)	(segid 3A4 and resid 319 and name CB)	5.08	0.08	0.08
	assign (segid 3A4 and resid 318 and name N)	(segid 3A4 and resid 319 and name N)	2.85	0.05	0.05
	assign (segid 3A4 and resid 318 and name N)	(segid 3A4 and resid 319 and name O)	5.03	0.26	0.26
65	assign (segid 3A4 and resid 318 and name N)	(segid 3A4 and resid 348 and name N)	7.09	0.74	0.75
	assign (segid 3A4 and resid 318 and name N)	(segid 3A4 and resid 383 and name C)	6.80	0.20	0.20
	assign (segid 3A4 and resid 318 and name N)	(segid 3A4 and resid 383 and name CA)	6.43	0.20	0.19
	assign (segid 3A4 and resid 318 and name N)	(segid 3A4 and resid 383 and name O)	6.13	0.23	0.23
	assign (segid 3A4 and resid 318 and name N)	(segid 3A4 and resid 433 and name C)	6.20	0.32	0.31
70	assign (segid 3A4 and resid 318 and name N)	(segid 3A4 and resid 433 and name CA)	6.15	0.28	0.28
	assign (segid 3A4 and resid 318 and name N)	(segid 3A4 and resid 433 and name N)	5.75	0.21	0.20
	assign (segid 3A4 and resid 318 and name N)	(segid 3A4 and resid 433 and name O)	5.62	0.35	0.34
	assign (segid 3A4 and resid 318 and name N)	(segid HEM and resid 1 and name C2B)	6.71	0.50	0.50
	assign (segid 3A4 and resid 318 and name N)	(segid HEM and resid 1 and name CMB)	5.37	0.51	0.51
75	assign (segid 3A4 and resid 318 and name O)	(segid 3A4 and resid 318 and name CB)	3.17	0.17	0.16
	assign (segid 3A4 and resid 318 and name O)	(segid 3A4 and resid 319 and name C)	3.62	0.23	0.24
	assign (segid 3A4 and resid 318 and name O)	(segid 3A4 and resid 319 and name CA)	2.74	0.03	0.03
	assign (segid 3A4 and resid 318 and name O)	(segid 3A4 and resid 319 and name CB)	3.94	0.16	0.15
	assign (segid 3A4 and resid 318 and name O)	(segid 3A4 and resid 319 and name N)	2.23	0.01	0.02
80	assign (segid 3A4 and resid 318 and name O)	(segid 3A4 and resid 319 and name O)	4.62	0.26	0.26
	assign (segid 3A4 and resid 318 and name O)	(segid 3A4 and resid 383 and name O)	7.69	0.09	0.09
	assign (segid 3A4 and resid 318 and name O)	(segid 3A4 and resid 431 and name C)	4.82	0.80	0.79
	assign (segid 3A4 and resid 318 and name O)	(segid 3A4 and resid 431 and name O)	4.47	1.03	1.04

	assign (segid 3A4 and resid 318 and name O) (segid 3A4 and resid 133 and name C)	4.70	0.30	0.31
	assign (segid 3A4 and resid 318 and name O) (segid 3A4 and resid 433 and name CA)	4.26	0.45	0.44
	assign (segid 3A4 and resid 318 and name O) (segid 3A4 and resid 433 and name N)	3.22	0.51	0.52
	assign (segid 3A4 and resid 318 and name O) (segid 3A4 and resid 433 and name O)	4.33	0.22	0.21
	assign (segid 3A4 and resid 318 and name O) (segid 3A4 and resid 434 and name CA)	6.73	0.49	0.50
5	assign (segid 3A4 and resid 318 and name O) (segid 3A4 and resid 434 and name N)	5.87	0.45	0.45
	assign (segid 3A4 and resid 318 and name O) (segid HEM and resid 1 and name CMB)	6.69	0.40	0.41
	assign (segid 3A4 and resid 318 and name O) (segid 3A4 and resid 319 and name CB)	2.52	0.02	0.01
	assign (segid 3A4 and resid 319 and name C) (segid 3A4 and resid 319 and name O)	1.23	0.00	0.00
	assign (segid 3A4 and resid 319 and name C) (segid 3A4 and resid 319 and name O)	6.82	0.45	0.44
10	assign (segid 3A4 and resid 319 and name C) (segid 3A4 and resid 345 and name O)	6.21	0.60	0.61
	assign (segid 3A4 and resid 319 and name C) (segid 3A4 and resid 347 and name C)	6.00	0.60	0.59
	assign (segid 3A4 and resid 319 and name C) (segid 3A4 and resid 347 and name CB)	5.08	0.50	0.50
	assign (segid 3A4 and resid 319 and name C) (segid 3A4 and resid 347 and name N)	5.90	0.70	0.70
	assign (segid 3A4 and resid 319 and name C) (segid 3A4 and resid 348 and name N)	5.69	0.74	0.74
15	assign (segid 3A4 and resid 319 and name C) (segid 3A4 and resid 382 and name O)	7.23	0.26	0.25
	assign (segid 3A4 and resid 319 and name C) (segid 3A4 and resid 383 and name C)	7.00	0.32	0.33
	assign (segid 3A4 and resid 319 and name C) (segid 3A4 and resid 383 and name CA)	7.06	0.29	0.29
	assign (segid 3A4 and resid 319 and name C) (segid 3A4 and resid 383 and name O)	6.12	0.39	0.39
20	assign (segid 3A4 and resid 319 and name C) (segid 3A4 and resid 433 and name N)	6.25	0.39	0.40
	assign (segid 3A4 and resid 319 and name C) (segid HEM and resid 1 and name C3A)	6.75	0.48	0.49
	assign (segid 3A4 and resid 319 and name C) (segid HEM and resid 1 and name CMA)	5.64	0.42	0.41
	assign (segid 3A4 and resid 319 and name C) (segid HEM and resid 1 and name C)	1.53	0.01	0.01
	assign (segid 3A4 and resid 319 and name CA) (segid 3A4 and resid 319 and name CB)	1.54	0.01	0.01
25	assign (segid 3A4 and resid 319 and name CA) (segid 3A4 and resid 319 and name O)	2.40	0.01	0.01
	assign (segid 3A4 and resid 319 and name CA) (segid 3A4 and resid 322 and name CA)	11.12	0.59	0.60
	assign (segid 3A4 and resid 319 and name CA) (segid 3A4 and resid 323 and name CA)	14.36	0.68	0.69
	assign (segid 3A4 and resid 319 and name CA) (segid 3A4 and resid 323 and name CB)	14.52	0.76	0.77
	assign (segid 3A4 and resid 319 and name CA) (segid 3A4 and resid 324 and name CA)	17.98	0.67	0.67
30	assign (segid 3A4 and resid 319 and name CA) (segid 3A4 and resid 324 and name CB)	18.56	0.73	0.73
	assign (segid 3A4 and resid 319 and name CA) (segid 3A4 and resid 342 and name CA)	17.51	0.66	0.65
	assign (segid 3A4 and resid 319 and name CA) (segid 3A4 and resid 343 and name CA)	15.24	0.61	0.61
	assign (segid 3A4 and resid 319 and name CA) (segid 3A4 and resid 343 and name CB)	15.67	0.55	0.54
	assign (segid 3A4 and resid 319 and name CA) (segid 3A4 and resid 344 and name CA)	11.75	0.61	0.61
	assign (segid 3A4 and resid 319 and name CA) (segid 3A4 and resid 344 and name CB)	11.63	0.62	0.62
35	assign (segid 3A4 and resid 319 and name CA) (segid 3A4 and resid 345 and name CA)	10.39	0.57	0.57
	assign (segid 3A4 and resid 319 and name CA) (segid 3A4 and resid 345 and name CB)	10.50	0.60	0.60
	assign (segid 3A4 and resid 319 and name CA) (segid 3A4 and resid 346 and name CA)	8.65	0.85	0.84
	assign (segid 3A4 and resid 319 and name CA) (segid 3A4 and resid 346 and name CB)	9.56	0.95	0.95
	assign (segid 3A4 and resid 319 and name CA) (segid 3A4 and resid 347 and name CA)	7.24	0.74	0.74
40	assign (segid 3A4 and resid 319 and name CA) (segid 3A4 and resid 347 and name CB)	6.16	0.69	0.69
	assign (segid 3A4 and resid 319 and name CA) (segid 3A4 and resid 348 and name CA)	7.56	0.90	0.91
	assign (segid 3A4 and resid 319 and name CA) (segid 3A4 and resid 349 and name CA)	11.04	0.89	0.89
	assign (segid 3A4 and resid 319 and name CA) (segid 3A4 and resid 349 and name CB)	11.59	0.89	0.89
	assign (segid 3A4 and resid 319 and name CA) (segid 3A4 and resid 350 and name CA)	11.96	0.56	0.56
45	assign (segid 3A4 and resid 319 and name CA) (segid 3A4 and resid 350 and name CB)	11.51	0.43	0.42
	assign (segid 3A4 and resid 319 and name CA) (segid 3A4 and resid 351 and name CA)	11.62	0.66	0.65
	assign (segid 3A4 and resid 319 and name CA) (segid 3A4 and resid 352 and name CA)	13.79	0.89	0.90
	assign (segid 3A4 and resid 319 and name CA) (segid 3A4 and resid 352 and name CB)	13.38	1.01	1.00
50	assign (segid 3A4 and resid 319 and name CA) (segid 3A4 and resid 353 and name CA)	16.27	0.83	0.83
	assign (segid 3A4 and resid 319 and name CA) (segid 3A4 and resid 353 and name CB)	16.18	0.80	0.80
	assign (segid 3A4 and resid 319 and name CA) (segid 3A4 and resid 356 and name CB)	17.96	0.83	0.83
	assign (segid 3A4 and resid 319 and name CA) (segid 3A4 and resid 357 and name CB)	17.49	0.62	0.62
	assign (segid 3A4 and resid 319 and name CA) (segid 3A4 and resid 360 and name CB)	17.44	0.77	0.78
55	assign (segid 3A4 and resid 319 and name CA) (segid 3A4 and resid 360 and name CA)	17.00	0.90	0.91
	assign (segid 3A4 and resid 319 and name CA) (segid 3A4 and resid 361 and name CB)	17.29	0.73	0.73
	assign (segid 3A4 and resid 319 and name CA) (segid 3A4 and resid 361 and name CB)	17.89	0.78	0.79
	assign (segid 3A4 and resid 319 and name CA) (segid 3A4 and resid 363 and name CA)	18.14	0.51	0.52
	assign (segid 3A4 and resid 319 and name CA) (segid 3A4 and resid 363 and name CB)	17.90	0.49	0.49
60	assign (segid 3A4 and resid 319 and name CA) (segid 3A4 and resid 381 and name CA)	12.51	0.37	0.37
	assign (segid 3A4 and resid 319 and name CA) (segid 3A4 and resid 382 and name CA)	9.93	0.31	0.31
	assign (segid 3A4 and resid 319 and name CA) (segid 3A4 and resid 382 and name CB)	10.10	0.36	0.35
	assign (segid 3A4 and resid 319 and name CA) (segid 3A4 and resid 383 and name C)	6.91	0.18	0.17
	assign (segid 3A4 and resid 319 and name CA) (segid 3A4 and resid 383 and name CA)	7.16	0.19	0.19
65	assign (segid 3A4 and resid 319 and name CA) (segid 3A4 and resid 383 and name O)	5.87	0.21	0.21
	assign (segid 3A4 and resid 319 and name CA) (segid 3A4 and resid 384 and name CA)	8.32	0.28	0.27
	assign (segid 3A4 and resid 319 and name CA) (segid 3A4 and resid 384 and name CB)	9.62	0.33	0.34
	assign (segid 3A4 and resid 319 and name CA) (segid 3A4 and resid 385 and name CA)	8.97	0.14	0.15
	assign (segid 3A4 and resid 319 and name CA) (segid 3A4 and resid 386 and name CA)	12.64	0.21	0.22
70	assign (segid 3A4 and resid 319 and name CA) (segid 3A4 and resid 387 and name CA)	15.47	0.39	0.38
	assign (segid 3A4 and resid 319 and name CA) (segid 3A4 and resid 388 and name CA)	16.79	0.24	0.23
	assign (segid 3A4 and resid 319 and name CA) (segid 3A4 and resid 388 and name CB)	17.83	0.41	0.41
	assign (segid 3A4 and resid 319 and name CA) (segid 3A4 and resid 389 and name CA)	13.65	0.30	0.31
	assign (segid 3A4 and resid 319 and name CA) (segid 3A4 and resid 389 and name CB)	13.10	0.46	0.47
75	assign (segid 3A4 and resid 319 and name CA) (segid 3A4 and resid 390 and name CA)	12.28	0.24	0.25
	assign (segid 3A4 and resid 319 and name CA) (segid 3A4 and resid 390 and name CB)	13.25	0.32	0.32
	assign (segid 3A4 and resid 319 and name CA) (segid 3A4 and resid 391 and name CA)	11.05	0.37	0.37
	assign (segid 3A4 and resid 319 and name CA) (segid 3A4 and resid 391 and name CB)	10.12	0.45	0.45
	assign (segid 3A4 and resid 319 and name CA) (segid 3A4 and resid 392 and name CA)	14.34	0.37	0.37
	assign (segid 3A4 and resid 319 and name CA) (segid 3A4 and resid 392 and name CB)	14.98	0.38	0.38
80	assign (segid 3A4 and resid 319 and name CA) (segid 3A4 and resid 393 and name CA)	13.72	0.54	0.54
	assign (segid 3A4 and resid 319 and name CA) (segid 3A4 and resid 394 and name CA)	13.01	0.45	0.45
	assign (segid 3A4 and resid 319 and name CA) (segid 3A4 and resid 394 and name CB)	13.09	0.44	0.43

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	assign (segid 3A4 and resid 319 and name CA) (segid 3A4 and resid 395 and name CA)	16.58	0.50	0.50
	assign (segid 3A4 and resid 319 and name CA) (segid 3A4 and resid 396 and name CA)	16.59	0.63	0.64
	assign (segid 3A4 and resid 319 and name CA) (segid 3A4 and resid 396 and name CB)	16.61	0.82	0.81
	assign (segid 3A4 and resid 319 and name CA) (segid 3A4 and resid 397 and name CA)	13.51	0.58	0.57
	assign (segid 3A4 and resid 319 and name CA) (segid 3A4 and resid 397 and name CB)	12.10	0.58	0.59
5	assign (segid 3A4 and resid 319 and name CA) (segid 3A4 and resid 398 and name CA)	15.23	0.48	0.47
	assign (segid 3A4 and resid 319 and name CA) (segid 3A4 and resid 398 and name CB)	15.58	0.52	0.53
	assign (segid 3A4 and resid 319 and name CA) (segid 3A4 and resid 399 and name CA)	18.50	0.44	0.44
	assign (segid 3A4 and resid 319 and name CA) (segid 3A4 and resid 400 and name CA)	17.56	0.50	0.49
	assign (segid 3A4 and resid 319 and name CA) (segid 3A4 and resid 400 and name CB)	16.66	0.55	0.55
10	assign (segid 3A4 and resid 319 and name CA) (segid 3A4 and resid 401 and name CA)	16.10	0.44	0.44
	assign (segid 3A4 and resid 319 and name CA) (segid 3A4 and resid 402 and name CA)	19.20	0.45	0.44
	assign (segid 3A4 and resid 319 and name CA) (segid 3A4 and resid 425 and name CA)	17.24	1.24	1.24
	assign (segid 3A4 and resid 319 and name CA) (segid 3A4 and resid 426 and name CA)	14.35	1.64	1.64
	assign (segid 3A4 and resid 319 and name CA) (segid 3A4 and resid 427 and name CA)	12.31	0.56	0.56
15	assign (segid 3A4 and resid 319 and name CA) (segid 3A4 and resid 428 and name CA)	11.97	1.30	1.30
	assign (segid 3A4 and resid 319 and name CA) (segid 3A4 and resid 429 and name CA)	10.29	1.26	1.27
	assign (segid 3A4 and resid 319 and name CA) (segid 3A4 and resid 430 and name CA)	9.10	1.47	1.48
	assign (segid 3A4 and resid 319 and name CA) (segid 3A4 and resid 431 and name CA)	6.54	1.22	1.23
	assign (segid 3A4 and resid 319 and name CA) (segid 3A4 and resid 433 and name C)	7.36	0.28	0.28
20	assign (segid 3A4 and resid 319 and name CA) (segid 3A4 and resid 433 and name CA)	6.77	0.37	0.38
	assign (segid 3A4 and resid 319 and name CA) (segid 3A4 and resid 433 and name N)	5.64	0.45	0.44
	assign (segid 3A4 and resid 319 and name CA) (segid 3A4 and resid 433 and name O)	6.95	0.22	0.23
	assign (segid 3A4 and resid 319 and name CA) (segid 3A4 and resid 434 and name CA)	9.41	0.51	0.51
	assign (segid 3A4 and resid 319 and name CA) (segid 3A4 and resid 435 and name CA)	12.89	0.48	0.49
25	assign (segid 3A4 and resid 319 and name CA) (segid 3A4 and resid 436 and name CA)	15.39	0.67	0.67
	assign (segid 3A4 and resid 319 and name CA) (segid 3A4 and resid 437 and name CA)	18.48	0.54	0.55
	assign (segid 3A4 and resid 319 and name CA) (segid 3A4 and resid 1 and name C2A)	7.31	0.29	0.28
	assign (segid 3A4 and resid 319 and name CA) (segid 3A4 and resid 1 and name C3A)	6.27	0.32	0.31
	assign (segid 3A4 and resid 319 and name CA) (segid 3A4 and resid 1 and name C4A)	6.50	0.44	0.43
30	assign (segid 3A4 and resid 319 and name CA) (segid 3A4 and resid 1 and name CHB)	5.98	0.53	0.53
	assign (segid 3A4 and resid 319 and name CA) (segid 3A4 and resid 1 and name CMA)	5.41	0.20	0.20
	assign (segid 3A4 and resid 319 and name CA) (segid 3A4 and resid 1 and name CMB)	5.90	0.59	0.58
	assign (segid 3A4 and resid 319 and name CB) (segid 3A4 and resid 322 and name CA)	10.74	0.62	0.63
35	assign (segid 3A4 and resid 319 and name CB) (segid 3A4 and resid 323 and name CA)	13.81	0.80	0.81
	assign (segid 3A4 and resid 319 and name CB) (segid 3A4 and resid 323 and name CB)	13.94	0.90	0.91
	assign (segid 3A4 and resid 319 and name CB) (segid 3A4 and resid 324 and name CA)	17.49	0.78	0.77
	assign (segid 3A4 and resid 319 and name CB) (segid 3A4 and resid 324 and name CB)	18.04	0.81	0.82
	assign (segid 3A4 and resid 319 and name CB) (segid 3A4 and resid 342 and name CA)	17.38	0.72	0.72
40	assign (segid 3A4 and resid 319 and name CB) (segid 3A4 and resid 343 and name CA)	15.16	0.69	0.68
	assign (segid 3A4 and resid 319 and name CB) (segid 3A4 and resid 343 and name CB)	15.49	0.66	0.67
	assign (segid 3A4 and resid 319 and name CB) (segid 3A4 and resid 344 and name CA)	11.85	0.66	0.67
	assign (segid 3A4 and resid 319 and name CB) (segid 3A4 and resid 344 and name CB)	11.89	0.65	0.66
	assign (segid 3A4 and resid 319 and name CB) (segid 3A4 and resid 345 and name CA)	10.38	0.72	0.73
	assign (segid 3A4 and resid 319 and name CB) (segid 3A4 and resid 345 and name CB)	10.30	0.79	0.80
45	assign (segid 3A4 and resid 319 and name CB) (segid 3A4 and resid 346 and name CA)	9.11	0.91	0.90
	assign (segid 3A4 and resid 319 and name CB) (segid 3A4 and resid 346 and name CB)	10.18	0.95	0.96
	assign (segid 3A4 and resid 319 and name CB) (segid 3A4 and resid 347 and name CA)	7.41	0.94	0.95
	assign (segid 3A4 and resid 319 and name CB) (segid 3A4 and resid 347 and name CB)	6.13	0.93	0.93
50	assign (segid 3A4 and resid 319 and name CB) (segid 3A4 and resid 348 and name CA)	8.36	1.02	1.02
	assign (segid 3A4 and resid 319 and name CB) (segid 3A4 and resid 349 and name CA)	11.77	0.98	0.98
	assign (segid 3A4 and resid 319 and name CB) (segid 3A4 and resid 349 and name CB)	12.31	0.96	0.96
	assign (segid 3A4 and resid 319 and name CB) (segid 3A4 and resid 350 and name CA)	12.26	0.72	0.72
	assign (segid 3A4 and resid 319 and name CB) (segid 3A4 and resid 350 and name CB)	11.63	0.61	0.62
	assign (segid 3A4 and resid 319 and name CB) (segid 3A4 and resid 351 and name CA)	11.98	0.72	0.73
55	assign (segid 3A4 and resid 319 and name CB) (segid 3A4 and resid 352 and name CA)	14.48	0.93	0.93
	assign (segid 3A4 and resid 319 and name CB) (segid 3A4 and resid 352 and name CB)	14.20	1.03	1.04
	assign (segid 3A4 and resid 319 and name CB) (segid 3A4 and resid 353 and name CA)	16.79	0.88	0.87
	assign (segid 3A4 and resid 319 and name CB) (segid 3A4 and resid 353 and name CB)	16.59	0.87	0.86
60	assign (segid 3A4 and resid 319 and name CB) (segid 3A4 and resid 357 and name CB)	17.86	0.69	0.70
	assign (segid 3A4 and resid 319 and name CB) (segid 3A4 and resid 361 and name CA)	18.25	0.71	0.70
	assign (segid 3A4 and resid 319 and name CB) (segid 3A4 and resid 363 and name CA)	18.84	0.47	0.47
	assign (segid 3A4 and resid 319 and name CB) (segid 3A4 and resid 363 and name CB)	18.63	0.46	0.46
	assign (segid 3A4 and resid 319 and name CB) (segid 3A4 and resid 381 and name CA)	12.24	0.51	0.51
	assign (segid 3A4 and resid 319 and name CB) (segid 3A4 and resid 382 and name CA)	9.41	0.45	0.45
65	assign (segid 3A4 and resid 319 and name CB) (segid 3A4 and resid 382 and name CB)	9.62	0.48	0.49
	assign (segid 3A4 and resid 319 and name CB) (segid 3A4 and resid 382 and name O)	7.11	0.45	0.44
	assign (segid 3A4 and resid 319 and name CB) (segid 3A4 and resid 383 and name C)	6.12	0.24	0.24
	assign (segid 3A4 and resid 319 and name CB) (segid 3A4 and resid 383 and name CA)	6.66	0.32	0.31
	assign (segid 3A4 and resid 319 and name CB) (segid 3A4 and resid 383 and name O)	5.00	0.22	0.23
70	assign (segid 3A4 and resid 319 and name CB) (segid 3A4 and resid 384 and name CA)	7.19	0.27	0.28
	assign (segid 3A4 and resid 319 and name CB) (segid 3A4 and resid 384 and name CB)	8.48	0.34	0.34
	assign (segid 3A4 and resid 319 and name CB) (segid 3A4 and resid 384 and name N)	7.12	0.25	0.24
	assign (segid 3A4 and resid 319 and name CB) (segid 3A4 and resid 385 and name CA)	7.87	0.25	0.25
	assign (segid 3A4 and resid 319 and name CB) (segid 3A4 and resid 385 and name N)	7.29	0.23	0.23
75	assign (segid 3A4 and resid 319 and name CB) (segid 3A4 and resid 386 and name CA)	11.57	0.29	0.30
	assign (segid 3A4 and resid 319 and name CB) (segid 3A4 and resid 387 and name CA)	14.29	0.45	0.44
	assign (segid 3A4 and resid 319 and name CB) (segid 3A4 and resid 388 and name CA)	15.15	0.29	0.29
	assign (segid 3A4 and resid 319 and name CB) (segid 3A4 and resid 388 and name CB)	16.50	0.45	0.46
80	assign (segid 3A4 and resid 319 and name CB) (segid 3A4 and resid 389 and name CA)	12.26	0.33	0.34
	assign (segid 3A4 and resid 319 and name CB) (segid 3A4 and resid 389 and name CB)	11.77	0.51	0.51
	assign (segid 3A4 and resid 319 and name CB) (segid 3A4 and resid 390 and name CA)	10.89	0.20	0.21
	assign (segid 3A4 and resid 319 and name CB) (segid 3A4 and resid 390 and name CB)	11.90	0.26	0.26

	assign (segid 3A4 and resid 319 and name CB)	(segid 3A4 and resid 391 and name CA)	9.58	0.35	0.36
	assign (segid 3A4 and resid 319 and name CB)	(segid 3A4 and resid 391 and name CB)	8.70	0.45	0.45
	assign (segid 3A4 and resid 319 and name CB)	(segid 3A4 and resid 392 and name CA)	12.88	0.36	0.36
	assign (segid 3A4 and resid 319 and name CB)	(segid 3A4 and resid 392 and name CB)	13.50	0.37	0.37
5	assign (segid 3A4 and resid 319 and name CB)	(segid 3A4 and resid 393 and name CA)	12.40	0.56	0.55
	assign (segid 3A4 and resid 319 and name CB)	(segid 3A4 and resid 394 and name CA)	11.81	0.47	0.48
	assign (segid 3A4 and resid 319 and name CB)	(segid 3A4 and resid 394 and name CB)	11.87	0.45	0.45
	assign (segid 3A4 and resid 319 and name CB)	(segid 3A4 and resid 395 and name CA)	15.45	0.51	0.52
	assign (segid 3A4 and resid 319 and name CB)	(segid 3A4 and resid 396 and name CA)	15.55	0.68	0.67
10	assign (segid 3A4 and resid 319 and name CB)	(segid 3A4 and resid 396 and name CB)	15.51	0.85	0.85
	assign (segid 3A4 and resid 319 and name CB)	(segid 3A4 and resid 397 and name CA)	12.63	0.61	0.62
	assign (segid 3A4 and resid 319 and name CB)	(segid 3A4 and resid 397 and name CB)	11.20	0.61	0.61
	assign (segid 3A4 and resid 319 and name CB)	(segid 3A4 and resid 398 and name CA)	14.49	0.50	0.49
	assign (segid 3A4 and resid 319 and name CB)	(segid 3A4 and resid 398 and name CB)	14.80	0.33	0.53
15	assign (segid 3A4 and resid 319 and name CB)	(segid 3A4 and resid 399 and name CA)	17.74	0.49	0.49
	assign (segid 3A4 and resid 319 and name CB)	(segid 3A4 and resid 399 and name CB)	18.39	0.54	0.55
	assign (segid 3A4 and resid 319 and name CB)	(segid 3A4 and resid 400 and name CA)	16.96	0.56	0.55
	assign (segid 3A4 and resid 319 and name CB)	(segid 3A4 and resid 400 and name CB)	16.04	0.62	0.62
	assign (segid 3A4 and resid 319 and name CB)	(segid 3A4 and resid 401 and name CA)	15.74	0.47	0.48
20	assign (segid 3A4 and resid 319 and name CB)	(segid 3A4 and resid 402 and name CA)	18.81	0.47	0.48
	assign (segid 3A4 and resid 319 and name CB)	(segid 3A4 and resid 402 and name CB)	19.15	0.47	0.48
	assign (segid 3A4 and resid 319 and name CB)	(segid 3A4 and resid 404 and name CB)	18.98	0.52	0.53
	assign (segid 3A4 and resid 319 and name CB)	(segid 3A4 and resid 426 and name CA)	15.69	1.60	1.60
	assign (segid 3A4 and resid 319 and name CB)	(segid 3A4 and resid 427 and name CA)	13.63	0.53	0.52
25	assign (segid 3A4 and resid 319 and name CB)	(segid 3A4 and resid 428 and name CA)	13.29	1.33	1.32
	assign (segid 3A4 and resid 319 and name CB)	(segid 3A4 and resid 429 and name CA)	11.54	1.33	1.32
	assign (segid 3A4 and resid 319 and name CB)	(segid 3A4 and resid 430 and name CA)	10.14	1.52	1.53
	assign (segid 3A4 and resid 319 and name CB)	(segid 3A4 and resid 431 and name CA)	7.28	1.40	1.40
	assign (segid 3A4 and resid 319 and name CB)	(segid 3A4 and resid 433 and name CA)	8.07	0.39	0.39
30	assign (segid 3A4 and resid 319 and name CB)	(segid 3A4 and resid 434 and name CA)	10.48	0.41	0.40
	assign (segid 3A4 and resid 319 and name CB)	(segid 3A4 and resid 435 and name CA)	13.96	0.44	0.43
	assign (segid 3A4 and resid 319 and name CB)	(segid 3A4 and resid 436 and name CA)	16.42	0.65	0.64
	assign (segid 3A4 and resid 319 and name CB)	(segid HEM and resid 1 and name C1A)	6.57	0.33	0.32
	assign (segid 3A4 and resid 319 and name CB)	(segid HEM and resid 1 and name C1B)	5.41	0.65	0.66
35	assign (segid 3A4 and resid 319 and name CB)	(segid HEM and resid 1 and name C2A)	5.84	0.25	0.24
	assign (segid 3A4 and resid 319 and name CB)	(segid HEM and resid 1 and name C2B)	5.65	0.68	0.67
	assign (segid 3A4 and resid 319 and name CB)	(segid HEM and resid 1 and name C3A)	4.81	0.27	0.27
	assign (segid 3A4 and resid 319 and name CB)	(segid HEM and resid 1 and name C4A)	5.04	0.44	0.44
	assign (segid 3A4 and resid 319 and name CB)	(segid HEM and resid 1 and name CAA)	6.50	0.22	0.22
40	assign (segid 3A4 and resid 319 and name CB)	(segid HEM and resid 1 and name CBA)	6.86	0.35	0.36
	assign (segid 3A4 and resid 319 and name CB)	(segid HEM and resid 1 and name CHB)	4.64	0.56	0.56
	assign (segid 3A4 and resid 319 and name CB)	(segid HEM and resid 1 and name CMA)	4.07	0.18	0.18
	assign (segid 3A4 and resid 319 and name CB)	(segid HEM and resid 1 and name CMB)	5.15	0.59	0.59
	assign (segid 3A4 and resid 319 and name CB)	(segid HEM and resid 1 and name NA)	6.16	0.43	0.44
45	assign (segid 3A4 and resid 319 and name CB)	(segid HEM and resid 1 and name NB)	6.48	0.67	0.66
	assign (segid 3A4 and resid 319 and name N)	(segid 3A4 and resid 319 and name C)	2.39	0.06	0.05
	assign (segid 3A4 and resid 319 and name N)	(segid 3A4 and resid 319 and name CA)	1.47	0.02	0.01
	assign (segid 3A4 and resid 319 and name N)	(segid 3A4 and resid 319 and name CB)	2.44	0.03	0.04
	assign (segid 3A4 and resid 319 and name N)	(segid 3A4 and resid 319 and name O)	3.02	0.16	0.16
50	assign (segid 3A4 and resid 319 and name N)	(segid 3A4 and resid 347 and name CB)	6.44	0.63	0.64
	assign (segid 3A4 and resid 319 and name N)	(segid 3A4 and resid 383 and name C)	6.58	0.14	0.13
	assign (segid 3A4 and resid 319 and name N)	(segid 3A4 and resid 383 and name CA)	6.66	0.16	0.17
	assign (segid 3A4 and resid 319 and name N)	(segid 3A4 and resid 383 and name O)	5.59	0.16	0.17
	assign (segid 3A4 and resid 319 and name N)	(segid 3A4 and resid 433 and name C)	6.66	0.25	0.25
55	assign (segid 3A4 and resid 319 and name N)	(segid 3A4 and resid 433 and name CA)	6.25	0.26	0.25
	assign (segid 3A4 and resid 319 and name N)	(segid 3A4 and resid 433 and name N)	5.28	0.31	0.32
	assign (segid 3A4 and resid 319 and name N)	(segid 3A4 and resid 433 and name O)	6.15	0.26	0.26
	assign (segid 3A4 and resid 319 and name N)	(segid HEM and resid 1 and name C1B)	6.51	0.55	0.55
	assign (segid 3A4 and resid 319 and name N)	(segid HEM and resid 1 and name C2B)	6.19	0.60	0.61
60	assign (segid 3A4 and resid 319 and name N)	(segid HEM and resid 1 and name C3A)	6.83	0.26	0.26
	assign (segid 3A4 and resid 319 and name N)	(segid HEM and resid 1 and name C4A)	6.85	0.37	0.38
	assign (segid 3A4 and resid 319 and name N)	(segid HEM and resid 1 and name CHB)	6.07	0.46	0.45
	assign (segid 3A4 and resid 319 and name N)	(segid HEM and resid 1 and name CMA)	5.99	0.15	0.15
	assign (segid 3A4 and resid 319 and name N)	(segid HEM and resid 1 and name CMB)	5.23	0.57	0.57
65	assign (segid 3A4 and resid 319 and name O)	(segid 3A4 and resid 319 and name CB)	2.86	0.12	0.12
	assign (segid 3A4 and resid 319 and name O)	(segid 3A4 and resid 345 and name O)	6.12	0.50	0.51
	assign (segid 3A4 and resid 319 and name O)	(segid 3A4 and resid 346 and name C)	6.11	0.93	0.93
	assign (segid 3A4 and resid 319 and name O)	(segid 3A4 and resid 346 and name CA)	6.51	0.92	0.93
	assign (segid 3A4 and resid 319 and name O)	(segid 3A4 and resid 347 and name C)	5.31	0.76	0.76
70	assign (segid 3A4 and resid 319 and name O)	(segid 3A4 and resid 347 and name CA)	5.00	0.68	0.69
	assign (segid 3A4 and resid 319 and name O)	(segid 3A4 and resid 347 and name CB)	4.05	0.53	0.52
	assign (segid 3A4 and resid 319 and name O)	(segid 3A4 and resid 347 and name N)	5.01	0.81	0.81
	assign (segid 3A4 and resid 319 and name O)	(segid 3A4 and resid 347 and name O)	6.27	0.67	0.67
	assign (segid 3A4 and resid 319 and name O)	(segid 3A4 and resid 348 and name CA)	5.81	0.94	0.95
75	assign (segid 3A4 and resid 319 and name O)	(segid 3A4 and resid 348 and name N)	4.94	0.94	0.94
	assign (segid 3A4 and resid 319 and name O)	(segid 3A4 and resid 382 and name C)	7.06	0.35	0.34
	assign (segid 3A4 and resid 319 and name O)	(segid 3A4 and resid 382 and name O)	6.18	0.32	0.33
	assign (segid 3A4 and resid 319 and name O)	(segid 3A4 and resid 383 and name C)	6.25	0.49	0.48
	assign (segid 3A4 and resid 319 and name O)	(segid 3A4 and resid 383 and name CA)	6.25	0.39	0.38
80	assign (segid 3A4 and resid 319 and name O)	(segid 3A4 and resid 383 and name N)	7.17	0.38	0.38
	assign (segid 3A4 and resid 319 and name O)	(segid 3A4 and resid 383 and name O)	5.47	0.57	0.56
	assign (segid 3A4 and resid 319 and name O)	(segid 3A4 and resid 385 and name N)	7.40	0.38	0.38
	assign (segid 3A4 and resid 319 and name O)	(segid HEM and resid 1 and name C3A)	6.39	0.66	0.65

	assign (segid 3A4 and resid 319 and name O)	(segid HEM and resid 1 and name C4A)	7.01	0.71	0.71
	assign (segid 3A4 and resid 319 and name O)	(segid HEM and resid 1 and name CHB)	6.66	0.77	0.76
	assign (segid 3A4 and resid 319 and name O)	(segid HEM and resid 1 and name CHA)	5.11	0.60	0.60
	assign (segid 3A4 and resid 31 and name C)	(segid 3A4 and resid 31 and name CB)	2.51	0.02	0.01
5	assign (segid 3A4 and resid 31 and name C)	(segid 3A4 and resid 31 and name O)	1.23	0.00	0.00
	assign (segid 3A4 and resid 31 and name C)	(segid 3A4 and resid 32 and name C)	3.40	0.06	0.07
	assign (segid 3A4 and resid 31 and name C)	(segid 3A4 and resid 32 and name CA)	2.43	0.02	0.02
	assign (segid 3A4 and resid 31 and name C)	(segid 3A4 and resid 32 and name CB)	3.52	0.06	0.06
	assign (segid 3A4 and resid 31 and name C)	(segid 3A4 and resid 32 and name N)	1.32	0.01	0.01
10	assign (segid 3A4 and resid 31 and name C)	(segid 3A4 and resid 32 and name O)	3.96	0.05	0.05
	assign (segid 3A4 and resid 31 and name C)	(segid 3A4 and resid 33 and name C)	6.46	0.12	0.13
	assign (segid 3A4 and resid 31 and name C)	(segid 3A4 and resid 33 and name CA)	5.38	0.15	0.14
	assign (segid 3A4 and resid 31 and name C)	(segid 3A4 and resid 33 and name CB)	5.94	0.21	0.20
	assign (segid 3A4 and resid 31 and name C)	(segid 3A4 and resid 33 and name N)	4.12	0.13	0.13
15	assign (segid 3A4 and resid 31 and name C)	(segid 3A4 and resid 33 and name O)	6.76	0.11	0.12
	assign (segid 3A4 and resid 31 and name C)	(segid 3A4 and resid 342 and name C)	5.34	0.08	0.08
	assign (segid 3A4 and resid 31 and name C)	(segid 3A4 and resid 342 and name CA)	6.77	0.08	0.09
	assign (segid 3A4 and resid 31 and name C)	(segid 3A4 and resid 342 and name N)	7.24	0.13	0.13
	assign (segid 3A4 and resid 31 and name C)	(segid 3A4 and resid 342 and name O)	4.48	0.09	0.10
20	assign (segid 3A4 and resid 31 and name C)	(segid 3A4 and resid 343 and name C)	4.76	0.14	0.15
	assign (segid 3A4 and resid 31 and name C)	(segid 3A4 and resid 343 and name CA)	4.38	0.14	0.14
	assign (segid 3A4 and resid 31 and name C)	(segid 3A4 and resid 343 and name CB)	5.03	0.21	0.21
	assign (segid 3A4 and resid 31 and name C)	(segid 3A4 and resid 343 and name N)	5.35	0.09	0.10
	assign (segid 3A4 and resid 31 and name C)	(segid 3A4 and resid 343 and name O)	5.96	0.14	0.15
25	assign (segid 3A4 and resid 31 and name C)	(segid 3A4 and resid 344 and name C)	5.23	0.18	0.17
	assign (segid 3A4 and resid 31 and name C)	(segid 3A4 and resid 344 and name CA)	4.98	0.21	0.22
	assign (segid 3A4 and resid 31 and name C)	(segid 3A4 and resid 344 and name CB)	4.93	0.35	0.35
	assign (segid 3A4 and resid 31 and name C)	(segid 3A4 and resid 344 and name N)	4.05	0.18	0.18
	assign (segid 3A4 and resid 31 and name C)	(segid 3A4 and resid 344 and name O)	4.54	0.16	0.17
30	assign (segid 3A4 and resid 31 and name C)	(segid 3A4 and resid 345 and name CA)	7.18	0.18	0.18
	assign (segid 3A4 and resid 31 and name C)	(segid 3A4 and resid 345 and name N)	6.47	0.18	0.19
	assign (segid 3A4 and resid 31 and name C)	(segid 3A4 and resid 34 and name N)	7.31	0.21	0.20
	assign (segid 3A4 and resid 31 and name CA)	(segid 3A4 and resid 319 and name CA)	17.58	0.59	0.59
35	assign (segid 3A4 and resid 31 and name CA)	(segid 3A4 and resid 319 and name CB)	17.84	0.60	0.59
	assign (segid 3A4 and resid 31 and name CA)	(segid 3A4 and resid 31 and name C)	1.53	0.01	0.01
	assign (segid 3A4 and resid 31 and name CA)	(segid 3A4 and resid 31 and name CB)	1.53	0.02	0.02
	assign (segid 3A4 and resid 31 and name CA)	(segid 3A4 and resid 31 and name O)	2.40	0.01	0.00
	assign (segid 3A4 and resid 31 and name CA)	(segid 3A4 and resid 322 and name CA)	9.88	0.38	0.37
40	assign (segid 3A4 and resid 31 and name CA)	(segid 3A4 and resid 323 and name CA)	9.85	0.12	0.12
	assign (segid 3A4 and resid 31 and name CA)	(segid 3A4 and resid 323 and name CB)	9.80	0.22	0.22
	assign (segid 3A4 and resid 31 and name CA)	(segid 3A4 and resid 324 and name CA)	9.93	0.20	0.20
	assign (segid 3A4 and resid 31 and name CA)	(segid 3A4 and resid 324 and name CB)	10.98	0.28	0.28
	assign (segid 3A4 and resid 31 and name CA)	(segid 3A4 and resid 325 and name CA)	10.54	0.32	0.32
45	assign (segid 3A4 and resid 31 and name CA)	(segid 3A4 and resid 325 and name CB)	9.82	0.42	0.42
	assign (segid 3A4 and resid 31 and name CA)	(segid 3A4 and resid 326 and name CA)	14.29	0.35	0.36
	assign (segid 3A4 and resid 31 and name CA)	(segid 3A4 and resid 326 and name CB)	15.35	0.35	0.35
	assign (segid 3A4 and resid 31 and name CA)	(segid 3A4 and resid 327 and name CA)	14.77	0.49	0.50
	assign (segid 3A4 and resid 31 and name CA)	(segid 3A4 and resid 327 and name CB)	15.91	0.54	0.55
	assign (segid 3A4 and resid 31 and name CA)	(segid 3A4 and resid 328 and name CA)	13.46	0.60	0.61
50	assign (segid 3A4 and resid 31 and name CA)	(segid 3A4 and resid 328 and name CB)	14.33	0.62	0.63
	assign (segid 3A4 and resid 31 and name CA)	(segid 3A4 and resid 329 and name CA)	12.54	0.70	0.71
	assign (segid 3A4 and resid 31 and name CA)	(segid 3A4 and resid 329 and name CB)	12.08	0.81	0.82
	assign (segid 3A4 and resid 31 and name CA)	(segid 3A4 and resid 32 and name C)	4.64	0.04	0.03
	assign (segid 3A4 and resid 31 and name CA)	(segid 3A4 and resid 32 and name CA)	3.81	0.01	0.02
55	assign (segid 3A4 and resid 31 and name CA)	(segid 3A4 and resid 32 and name CB)	4.75	0.03	0.02
	assign (segid 3A4 and resid 31 and name CA)	(segid 3A4 and resid 32 and name N)	2.44	0.02	0.02
	assign (segid 3A4 and resid 31 and name CA)	(segid 3A4 and resid 32 and name O)	4.92	0.07	0.06
	assign (segid 3A4 and resid 31 and name CA)	(segid 3A4 and resid 330 and name CA)	12.35	0.48	0.48
	assign (segid 3A4 and resid 31 and name CA)	(segid 3A4 and resid 330 and name CB)	13.66	0.47	0.46
60	assign (segid 3A4 and resid 31 and name CA)	(segid 3A4 and resid 331 and name CA)	10.78	0.44	0.44
	assign (segid 3A4 and resid 31 and name CA)	(segid 3A4 and resid 331 and name CB)	9.49	0.44	0.43
	assign (segid 3A4 and resid 31 and name CA)	(segid 3A4 and resid 332 and name CA)	12.50	0.54	0.54
	assign (segid 3A4 and resid 31 and name CA)	(segid 3A4 and resid 333 and name CA)	13.60	0.89	0.89
	assign (segid 3A4 and resid 31 and name CA)	(segid 3A4 and resid 335 and name CA)	10.11	0.40	0.40
65	assign (segid 3A4 and resid 31 and name CA)	(segid 3A4 and resid 336 and name CA)	10.59	0.38	0.38
	assign (segid 3A4 and resid 31 and name CA)	(segid 3A4 and resid 336 and name CB)	11.77	0.34	0.35
	assign (segid 3A4 and resid 31 and name CA)	(segid 3A4 and resid 337 and name CA)	8.40	0.64	0.63
	assign (segid 3A4 and resid 31 and name CA)	(segid 3A4 and resid 337 and name CB)	7.77	0.71	0.72
	assign (segid 3A4 and resid 31 and name CA)	(segid 3A4 and resid 338 and name CA)	10.60	0.58	0.58
70	assign (segid 3A4 and resid 31 and name CA)	(segid 3A4 and resid 338 and name CB)	10.87	0.67	0.68
	assign (segid 3A4 and resid 31 and name CA)	(segid 3A4 and resid 339 and name CA)	12.39	0.49	0.48
	assign (segid 3A4 and resid 31 and name CA)	(segid 3A4 and resid 339 and name CB)	13.91	0.48	0.48
	assign (segid 3A4 and resid 31 and name CA)	(segid 3A4 and resid 33 and name C)	7.74	0.12	0.12
	assign (segid 3A4 and resid 31 and name CA)	(segid 3A4 and resid 33 and name CA)	6.54	0.12	0.13
75	assign (segid 3A4 and resid 31 and name CA)	(segid 3A4 and resid 33 and name CB)	7.03	0.17	0.17
	assign (segid 3A4 and resid 31 and name CA)	(segid 3A4 and resid 33 and name N)	5.41	0.11	0.12
	assign (segid 3A4 and resid 31 and name CA)	(segid 3A4 and resid 340 and name CA)	11.43	0.21	0.21
	assign (segid 3A4 and resid 31 and name CA)	(segid 3A4 and resid 341 and name C)	7.21	0.17	0.17
	assign (segid 3A4 and resid 31 and name CA)	(segid 3A4 and resid 341 and name CA)	7.68	0.23	0.24
80	assign (segid 3A4 and resid 31 and name CA)	(segid 3A4 and resid 341 and name CB)	6.95	0.34	0.33
	assign (segid 3A4 and resid 31 and name CA)	(segid 3A4 and resid 342 and name C)	5.08	0.12	0.12
	assign (segid 3A4 and resid 31 and name CA)	(segid 3A4 and resid 342 and name CA)	6.39	0.09	0.10
	assign (segid 3A4 and resid 31 and name CA)	(segid 3A4 and resid 342 and name N)	6.57	0.13	0.12

	assign (segid 3A4 and resid 31 and name CB) (segid 3A4 and resid 33 and name CA)	6.50	0.16	0.17
	assign (segid 3A4 and resid 31 and name CB) (segid 3A4 and resid 33 and name CB)	6.75	0.19	0.18
	assign (segid 3A4 and resid 31 and name CB) (segid 3A4 and resid 33 and name N)	5.61	0.17	0.18
	assign (segid 3A4 and resid 31 and name CB) (segid 3A4 and resid 340 and name CA)	10.82	0.24	0.25
5	assign (segid 3A4 and resid 31 and name CB) (segid 3A4 and resid 341 and name C)	6.77	0.18	0.17
	assign (segid 3A4 and resid 31 and name CB) (segid 3A4 and resid 341 and name CA)	7.16	0.22	0.23
	assign (segid 3A4 and resid 31 and name CB) (segid 3A4 and resid 341 and name CB)	6.23	0.32	0.32
	assign (segid 3A4 and resid 31 and name CB) (segid 3A4 and resid 341 and name CG)	6.86	0.37	0.37
	assign (segid 3A4 and resid 31 and name CB) (segid 3A4 and resid 341 and name O)	7.13	0.23	0.23
10	assign (segid 3A4 and resid 31 and name CB) (segid 3A4 and resid 342 and name C)	5.05	0.29	0.29
	assign (segid 3A4 and resid 31 and name CB) (segid 3A4 and resid 342 and name CA)	6.37	0.24	0.23
	assign (segid 3A4 and resid 31 and name CB) (segid 3A4 and resid 342 and name N)	6.39	0.20	0.20
	assign (segid 3A4 and resid 31 and name CB) (segid 3A4 and resid 342 and name O)	4.06	0.27	0.26
	assign (segid 3A4 and resid 31 and name CB) (segid 3A4 and resid 343 and name C)	5.65	0.40	0.40
	assign (segid 3A4 and resid 31 and name CB) (segid 3A4 and resid 343 and name CA)	4.62	0.43	0.43
15	assign (segid 3A4 and resid 31 and name CB) (segid 3A4 and resid 343 and name CB)	4.83	0.58	0.58
	assign (segid 3A4 and resid 31 and name CB) (segid 3A4 and resid 343 and name N)	5.32	0.36	0.35
	assign (segid 3A4 and resid 31 and name CB) (segid 3A4 and resid 343 and name O)	6.80	0.42	0.42
	assign (segid 3A4 and resid 31 and name CB) (segid 3A4 and resid 344 and name C)	7.00	0.33	0.33
20	assign (segid 3A4 and resid 31 and name CB) (segid 3A4 and resid 344 and name CA)	6.74	0.37	0.37
	assign (segid 3A4 and resid 31 and name CB) (segid 3A4 and resid 344 and name CB)	7.01	0.43	0.43
	assign (segid 3A4 and resid 31 and name CB) (segid 3A4 and resid 344 and name N)	5.48	0.38	0.38
	assign (segid 3A4 and resid 31 and name CB) (segid 3A4 and resid 344 and name O)	6.40	0.30	0.30
	assign (segid 3A4 and resid 31 and name CB) (segid 3A4 and resid 345 and name CA)	8.76	0.34	0.34
25	assign (segid 3A4 and resid 31 and name CB) (segid 3A4 and resid 345 and name CB)	9.51	0.46	0.46
	assign (segid 3A4 and resid 31 and name CB) (segid 3A4 and resid 346 and name CA)	11.06	0.30	0.31
	assign (segid 3A4 and resid 31 and name CB) (segid 3A4 and resid 346 and name CB)	10.85	0.37	0.37
	assign (segid 3A4 and resid 31 and name CB) (segid 3A4 and resid 347 and name CA)	14.34	0.28	0.28
	assign (segid 3A4 and resid 31 and name CB) (segid 3A4 and resid 347 and name CB)	15.19	0.26	0.26
	assign (segid 3A4 and resid 31 and name CB) (segid 3A4 and resid 347 and name N)	16.27	0.33	0.33
30	assign (segid 3A4 and resid 31 and name CB) (segid 3A4 and resid 348 and name CA)	14.64	0.41	0.41
	assign (segid 3A4 and resid 31 and name CB) (segid 3A4 and resid 349 and name CA)	13.29	0.40	0.39
	assign (segid 3A4 and resid 31 and name CB) (segid 3A4 and resid 349 and name CB)	9.94	0.24	0.23
	assign (segid 3A4 and resid 31 and name CB) (segid 3A4 and resid 34 and name CB)	10.23	0.26	0.26
	assign (segid 3A4 and resid 31 and name CB) (segid 3A4 and resid 34 and name CA)	15.32	0.77	0.77
35	assign (segid 3A4 and resid 31 and name CB) (segid 3A4 and resid 350 and name CB)	15.03	0.88	0.87
	assign (segid 3A4 and resid 31 and name CB) (segid 3A4 and resid 350 and name CA)	12.29	0.32	0.33
	assign (segid 3A4 and resid 31 and name CB) (segid 3A4 and resid 35 and name CA)	14.58	0.21	0.21
	assign (segid 3A4 and resid 31 and name CB) (segid 3A4 and resid 36 and name CA)	14.47	0.23	0.24
40	assign (segid 3A4 and resid 31 and name CB) (segid 3A4 and resid 37 and name CA)	14.90	0.34	0.34
	assign (segid 3A4 and resid 31 and name CB) (segid 3A4 and resid 37 and name CB)	18.60	0.51	0.50
	assign (segid 3A4 and resid 31 and name CB) (segid 3A4 and resid 382 and name CA)	17.17	0.52	0.53
	assign (segid 3A4 and resid 31 and name CB) (segid 3A4 and resid 382 and name CB)	17.71	0.27	0.28
	assign (segid 3A4 and resid 31 and name CB) (segid 3A4 and resid 385 and name CA)	17.86	0.26	0.25
45	assign (segid 3A4 and resid 31 and name CB) (segid 3A4 and resid 386 and name CA)	19.25	0.64	0.64
	assign (segid 3A4 and resid 31 and name CB) (segid 3A4 and resid 389 and name CA)	18.01	0.66	0.66
	assign (segid 3A4 and resid 31 and name CB) (segid 3A4 and resid 389 and name CB)	10.81	0.21	0.21
	assign (segid 3A4 and resid 31 and name CB) (segid 3A4 and resid 38 and name CB)	9.75	0.29	0.29
	assign (segid 3A4 and resid 31 and name CB) (segid 3A4 and resid 39 and name CA)	11.12	0.14	0.13
50	assign (segid 3A4 and resid 31 and name CB) (segid 3A4 and resid 39 and name CB)	11.70	0.18	0.17
	assign (segid 3A4 and resid 31 and name CB) (segid 3A4 and resid 39 and name N)	14.34	0.14	0.13
	assign (segid 3A4 and resid 31 and name CB) (segid 3A4 and resid 40 and name CB)	15.54	0.15	0.16
	assign (segid 3A4 and resid 31 and name CB) (segid 3A4 and resid 40 and name CA)	13.10	0.30	0.31
	assign (segid 3A4 and resid 31 and name CB) (segid 3A4 and resid 41 and name CB)	12.59	0.38	0.39
	assign (segid 3A4 and resid 31 and name CB) (segid 3A4 and resid 41 and name CA)	10.49	0.21	0.20
55	assign (segid 3A4 and resid 31 and name CB) (segid 3A4 and resid 42 and name CB)	9.22	0.19	0.18
	assign (segid 3A4 and resid 31 and name CB) (segid 3A4 and resid 31 and name C)	2.40	0.04	0.03
	assign (segid 3A4 and resid 31 and name N) (segid 3A4 and resid 31 and name CA)	1.45	0.01	0.01
	assign (segid 3A4 and resid 31 and name N) (segid 3A4 and resid 31 and name CB)	2.44	0.03	0.03
	assign (segid 3A4 and resid 31 and name N) (segid 3A4 and resid 31 and name O)	2.73	0.07	0.07
60	assign (segid 3A4 and resid 31 and name N) (segid 3A4 and resid 323 and name O)	7.52	0.11	0.11
	assign (segid 3A4 and resid 31 and name N) (segid 3A4 and resid 32 and name C)	5.78	0.07	0.07
	assign (segid 3A4 and resid 31 and name N) (segid 3A4 and resid 32 and name CA)	4.73	0.05	0.05
	assign (segid 3A4 and resid 31 and name N) (segid 3A4 and resid 32 and name CB)	5.52	0.05	0.05
	assign (segid 3A4 and resid 31 and name N) (segid 3A4 and resid 32 and name N)	3.51	0.05	0.04
65	assign (segid 3A4 and resid 31 and name N) (segid 3A4 and resid 32 and name O)	6.20	0.06	0.06
	assign (segid 3A4 and resid 31 and name N) (segid 3A4 and resid 33 and name CA)	7.69	0.16	0.16
	assign (segid 3A4 and resid 31 and name N) (segid 3A4 and resid 33 and name N)	6.47	0.14	0.15
	assign (segid 3A4 and resid 31 and name N) (segid 3A4 and resid 341 and name C)	6.27	0.21	0.21
	assign (segid 3A4 and resid 31 and name N) (segid 3A4 and resid 341 and name CA)	6.78	0.26	0.26
70	assign (segid 3A4 and resid 31 and name N) (segid 3A4 and resid 341 and name CB)	6.24	0.36	0.36
	assign (segid 3A4 and resid 31 and name N) (segid 3A4 and resid 341 and name CG)	6.93	0.34	0.34
	assign (segid 3A4 and resid 31 and name N) (segid 3A4 and resid 341 and name O)	6.89	0.25	0.26
	assign (segid 3A4 and resid 31 and name N) (segid 3A4 and resid 342 and name C)	4.14	0.09	0.09
75	assign (segid 3A4 and resid 31 and name N) (segid 3A4 and resid 342 and name CA)	5.31	0.09	0.09
	assign (segid 3A4 and resid 31 and name N) (segid 3A4 and resid 342 and name N)	5.47	0.15	0.14
	assign (segid 3A4 and resid 31 and name N) (segid 3A4 and resid 342 and name O)	3.01	0.09	0.08
	assign (segid 3A4 and resid 31 and name N) (segid 3A4 and resid 343 and name C)	5.19	0.21	0.21
	assign (segid 3A4 and resid 31 and name N) (segid 3A4 and resid 343 and name CA)	4.40	0.21	0.20
80	assign (segid 3A4 and resid 31 and name N) (segid 3A4 and resid 343 and name CB)	5.32	0.28	0.27
	assign (segid 3A4 and resid 31 and name N) (segid 3A4 and resid 343 and name N)	4.73	0.15	0.15
	assign (segid 3A4 and resid 31 and name N) (segid 3A4 and resid 343 and name O)	6.30	0.19	0.19
	assign (segid 3A4 and resid 31 and name N) (segid 3A4 and resid 344 and name C)	6.81	0.19	0.18

	assign (segid 3A4 and resid 31 and name N) (segid 3A4 and resid 344 and name CA)	6.10	0.27	0.26
	assign (segid 3A4 and resid 31 and name N) (segid 3A4 and resid 344 and name CB)	5.96	0.36	0.37
	assign (segid 3A4 and resid 31 and name N) (segid 3A4 and resid 344 and name N)	4.94	0.24	0.24
	assign (segid 3A4 and resid 31 and name N) (segid 3A4 and resid 344 and name O)	6.43	0.13	0.13
5	assign (segid 3A4 and resid 31 and name O) (segid 3A4 and resid 31 and name CB)	3.13	0.06	0.07
	assign (segid 3A4 and resid 31 and name O) (segid 3A4 and resid 323 and name N)	7.65	0.10	0.10
	assign (segid 3A4 and resid 31 and name O) (segid 3A4 and resid 323 and name O)	7.08	0.08	0.08
	assign (segid 3A4 and resid 31 and name O) (segid 3A4 and resid 32 and name C)	3.76	0.13	0.13
	assign (segid 3A4 and resid 31 and name O) (segid 3A4 and resid 32 and name CA)	2.76	0.04	0.04
10	assign (segid 3A4 and resid 31 and name O) (segid 3A4 and resid 32 and name CB)	3.91	0.13	0.13
	assign (segid 3A4 and resid 31 and name O) (segid 3A4 and resid 32 and name N)	2.24	0.02	0.01
	assign (segid 3A4 and resid 31 and name O) (segid 3A4 and resid 32 and name O)	4.58	0.10	0.11
	assign (segid 3A4 and resid 31 and name O) (segid 3A4 and resid 33 and name C)	6.47	0.22	0.21
	assign (segid 3A4 and resid 31 and name O) (segid 3A4 and resid 33 and name CA)	5.43	0.29	0.28
	assign (segid 3A4 and resid 31 and name O) (segid 3A4 and resid 33 and name CB)	5.77	0.38	0.39
15	assign (segid 3A4 and resid 31 and name O) (segid 3A4 and resid 33 and name N)	4.13	0.23	0.24
	assign (segid 3A4 and resid 31 and name O) (segid 3A4 and resid 33 and name O)	6.58	0.14	0.14
	assign (segid 3A4 and resid 31 and name O) (segid 3A4 and resid 341 and name C)	7.50	0.22	0.23
	assign (segid 3A4 and resid 31 and name O) (segid 3A4 and resid 341 and name O)	7.75	0.28	0.28
20	assign (segid 3A4 and resid 31 and name O) (segid 3A4 and resid 342 and name C)	4.64	0.12	0.12
	assign (segid 3A4 and resid 31 and name O) (segid 3A4 and resid 342 and name CA)	6.11	0.13	0.12
	assign (segid 3A4 and resid 31 and name O) (segid 3A4 and resid 342 and name N)	6.77	0.16	0.16
	assign (segid 3A4 and resid 31 and name O) (segid 3A4 and resid 342 and name O)	4.00	0.17	0.17
	assign (segid 3A4 and resid 31 and name O) (segid 3A4 and resid 343 and name C)	3.62	0.11	0.11
25	assign (segid 3A4 and resid 31 and name O) (segid 3A4 and resid 343 and name CA)	3.41	0.05	0.05
	assign (segid 3A4 and resid 31 and name O) (segid 3A4 and resid 343 and name CB)	4.20	0.02	0.03
	assign (segid 3A4 and resid 31 and name O) (segid 3A4 and resid 343 and name N)	4.46	0.08	0.07
	assign (segid 3A4 and resid 31 and name O) (segid 3A4 and resid 343 and name O)	4.82	0.11	0.11
	assign (segid 3A4 and resid 31 and name O) (segid 3A4 and resid 344 and name C)	4.27	0.20	0.21
30	assign (segid 3A4 and resid 31 and name O) (segid 3A4 and resid 344 and name CA)	3.88	0.24	0.23
	assign (segid 3A4 and resid 31 and name O) (segid 3A4 and resid 344 and name CB)	3.97	0.38	0.37
	assign (segid 3A4 and resid 31 and name O) (segid 3A4 and resid 344 and name N)	2.88	0.18	0.17
	assign (segid 3A4 and resid 31 and name O) (segid 3A4 and resid 344 and name O)	3.79	0.19	0.19
	assign (segid 3A4 and resid 31 and name O) (segid 3A4 and resid 345 and name C)	7.29	0.30	0.30
35	assign (segid 3A4 and resid 31 and name O) (segid 3A4 and resid 345 and name CA)	6.36	0.23	0.24
	assign (segid 3A4 and resid 31 and name O) (segid 3A4 and resid 345 and name CB)	7.36	0.20	0.20
	assign (segid 3A4 and resid 31 and name O) (segid 3A4 and resid 345 and name N)	5.52	0.23	0.22
	assign (segid 3A4 and resid 31 and name O) (segid 3A4 and resid 346 and name N)	7.36	0.29	0.30
	assign (segid 3A4 and resid 31 and name O) (segid 3A4 and resid 34 and name N)	7.47	0.26	0.25
40	assign (segid 3A4 and resid 31 and name O) (segid 3A4 and resid 322 and name O)	1.23	0.01	0.02
	assign (segid 3A4 and resid 322 and name C) (segid 3A4 and resid 322 and name O)	3.57	0.06	0.07
	assign (segid 3A4 and resid 322 and name C) (segid 3A4 and resid 323 and name C)	2.46	0.01	0.00
	assign (segid 3A4 and resid 322 and name C) (segid 3A4 and resid 323 and name CA)	3.37	0.09	0.09
	assign (segid 3A4 and resid 322 and name C) (segid 3A4 and resid 323 and name CB)	3.54	0.19	0.18
	assign (segid 3A4 and resid 322 and name C) (segid 3A4 and resid 323 and name CG)	1.33	0.00	0.01
45	assign (segid 3A4 and resid 322 and name C) (segid 3A4 and resid 323 and name N)	3.85	0.09	0.10
	assign (segid 3A4 and resid 322 and name C) (segid 3A4 and resid 323 and name O)	6.98	0.05	0.05
	assign (segid 3A4 and resid 322 and name C) (segid 3A4 and resid 324 and name C)	5.91	0.10	0.09
	assign (segid 3A4 and resid 322 and name C) (segid 3A4 and resid 324 and name CA)	6.51	0.23	0.23
	assign (segid 3A4 and resid 322 and name C) (segid 3A4 and resid 324 and name CB)	4.64	0.07	0.08
50	assign (segid 3A4 and resid 322 and name C) (segid 3A4 and resid 324 and name N)	7.15	0.10	0.10
	assign (segid 3A4 and resid 322 and name C) (segid 3A4 and resid 325 and name N)	7.91	0.06	0.06
	assign (segid 3A4 and resid 322 and name C) (segid 3A4 and resid 342 and name C)	6.63	0.09	0.09
	assign (segid 3A4 and resid 322 and name C) (segid 3A4 and resid 342 and name CA)	6.79	0.18	0.17
	assign (segid 3A4 and resid 322 and name C) (segid 3A4 and resid 342 and name O)	7.67	0.10	0.10
55	assign (segid 3A4 and resid 322 and name C) (segid 3A4 and resid 343 and name C)	4.85	0.11	0.12
	assign (segid 3A4 and resid 322 and name C) (segid 3A4 and resid 343 and name CA)	5.77	0.08	0.08
	assign (segid 3A4 and resid 322 and name C) (segid 3A4 and resid 343 and name CB)	6.03	0.14	0.14
	assign (segid 3A4 and resid 322 and name C) (segid 3A4 and resid 343 and name N)	5.57	0.05	0.06
60	assign (segid 3A4 and resid 322 and name C) (segid 3A4 and resid 343 and name O)	3.65	0.11	0.10
	assign (segid 3A4 and resid 322 and name C) (segid 3A4 and resid 344 and name C)	6.23	0.32	0.33
	assign (segid 3A4 and resid 322 and name C) (segid 3A4 and resid 344 and name CA)	5.54	0.14	0.14
	assign (segid 3A4 and resid 322 and name C) (segid 3A4 and resid 344 and name CB)	6.51	0.21	0.21
	assign (segid 3A4 and resid 322 and name C) (segid 3A4 and resid 344 and name N)	5.69	0.13	0.13
65	assign (segid 3A4 and resid 322 and name C) (segid 3A4 and resid 345 and name N)	5.91	0.43	0.43
	assign (segid 3A4 and resid 322 and name CA) (segid 3A4 and resid 322 and name C)	1.52	0.01	0.01
	assign (segid 3A4 and resid 322 and name CA) (segid 3A4 and resid 322 and name O)	2.40	0.02	0.01
	assign (segid 3A4 and resid 322 and name CA) (segid 3A4 and resid 323 and name C)	4.70	0.05	0.05
	assign (segid 3A4 and resid 322 and name CA) (segid 3A4 and resid 323 and name CA)	3.79	0.02	0.01
70	assign (segid 3A4 and resid 322 and name CA) (segid 3A4 and resid 323 and name CB)	4.58	0.09	0.09
	assign (segid 3A4 and resid 322 and name CA) (segid 3A4 and resid 323 and name N)	4.67	0.21	0.20
	assign (segid 3A4 and resid 322 and name CA) (segid 3A4 and resid 323 and name O)	2.39	0.02	0.02
	assign (segid 3A4 and resid 322 and name CA) (segid 3A4 and resid 323 and name O)	4.64	0.07	0.08
	assign (segid 3A4 and resid 322 and name CA) (segid 3A4 and resid 324 and name CA)	7.03	0.10	0.10
	assign (segid 3A4 and resid 322 and name CA) (segid 3A4 and resid 324 and name CB)	7.62	0.25	0.25
75	assign (segid 3A4 and resid 322 and name CA) (segid 3A4 and resid 324 and name N)	5.89	0.08	0.08
	assign (segid 3A4 and resid 322 and name CA) (segid 3A4 and resid 325 and name CA)	10.21	0.12	0.12
	assign (segid 3A4 and resid 322 and name CA) (segid 3A4 and resid 325 and name CB)	10.92	0.21	0.22
	assign (segid 3A4 and resid 322 and name CA) (segid 3A4 and resid 326 and name CA)	12.98	0.12	0.12
80	assign (segid 3A4 and resid 322 and name CA) (segid 3A4 and resid 326 and name CB)	13.28	0.10	0.09
	assign (segid 3A4 and resid 322 and name CA) (segid 3A4 and resid 327 and name CA)	15.66	0.29	0.28
	assign (segid 3A4 and resid 322 and name CA) (segid 3A4 and resid 327 and name CB)	16.57	0.34	0.33
	assign (segid 3A4 and resid 322 and name CA) (segid 3A4 and resid 328 and name CA)	16.68	0.41	0.41

	assign (segid 3A4 and resid 322 and name CA) (segid 3A4 and resid 328 and name CB)	18.07	0.40	0.39
	assign (segid 3A4 and resid 322 and name CA) (segid 3A4 and resid 329 and name CA)	16.00	0.75	0.75
	assign (segid 3A4 and resid 322 and name CA) (segid 3A4 and resid 329 and name CB)	14.77	0.81	0.81
	assign (segid 3A4 and resid 322 and name CA) (segid 3A4 and resid 330 and name CA)	17.34	0.85	0.85
	assign (segid 3A4 and resid 322 and name CA) (segid 3A4 and resid 331 and name CA)	15.56	0.85	0.84
5	assign (segid 3A4 and resid 322 and name CA) (segid 3A4 and resid 331 and name CB)	14.09	0.85	0.85
	assign (segid 3A4 and resid 322 and name CA) (segid 3A4 and resid 336 and name CA)	17.46	0.54	0.55
	assign (segid 3A4 and resid 322 and name CA) (segid 3A4 and resid 337 and name CA)	14.27	0.50	0.51
	assign (segid 3A4 and resid 322 and name CA) (segid 3A4 and resid 337 and name CB)	13.03	0.54	0.53
	assign (segid 3A4 and resid 322 and name CA) (segid 3A4 and resid 338 and name CA)	15.35	0.25	0.24
10	assign (segid 3A4 and resid 322 and name CA) (segid 3A4 and resid 338 and name CB)	16.03	0.25	0.25
	assign (segid 3A4 and resid 322 and name CA) (segid 3A4 and resid 339 and name CA)	14.53	0.10	0.11
	assign (segid 3A4 and resid 322 and name CA) (segid 3A4 and resid 339 and name CB)	15.75	0.11	0.11
	assign (segid 3A4 and resid 322 and name CA) (segid 3A4 and resid 340 and name CA)	12.22	0.37	0.38
	assign (segid 3A4 and resid 322 and name CA) (segid 3A4 and resid 341 and name CA)	10.54	0.18	0.18
15	assign (segid 3A4 and resid 322 and name CA) (segid 3A4 and resid 341 and name CB)	11.11	0.20	0.21
	assign (segid 3A4 and resid 322 and name CA) (segid 3A4 and resid 342 and name C)	6.72	0.10	0.10
	assign (segid 3A4 and resid 322 and name CA) (segid 3A4 and resid 342 and name CA)	7.03	0.18	0.18
	assign (segid 3A4 and resid 322 and name CA) (segid 3A4 and resid 342 and name O)	7.63	0.11	0.11
	assign (segid 3A4 and resid 322 and name CA) (segid 3A4 and resid 343 and name C)	4.55	0.27	0.26
20	assign (segid 3A4 and resid 322 and name CA) (segid 3A4 and resid 343 and name CA)	5.74	0.20	0.20
	assign (segid 3A4 and resid 322 and name CA) (segid 3A4 and resid 343 and name CB)	6.25	0.25	0.25
	assign (segid 3A4 and resid 322 and name CA) (segid 3A4 and resid 343 and name N)	5.71	0.11	0.12
	assign (segid 3A4 and resid 322 and name CA) (segid 3A4 and resid 343 and name O)	3.41	0.24	0.24
	assign (segid 3A4 and resid 322 and name CA) (segid 3A4 and resid 344 and name C)	5.39	0.53	0.54
25	assign (segid 3A4 and resid 322 and name CA) (segid 3A4 and resid 344 and name CA)	4.64	0.32	0.32
	assign (segid 3A4 and resid 322 and name CA) (segid 3A4 and resid 344 and name CB)	5.42	0.21	0.21
	assign (segid 3A4 and resid 322 and name CA) (segid 3A4 and resid 344 and name N)	5.09	0.30	0.30
	assign (segid 3A4 and resid 322 and name CA) (segid 3A4 and resid 344 and name O)	6.55	0.52	0.53
	assign (segid 3A4 and resid 322 and name CA) (segid 3A4 and resid 345 and name CA)	6.26	0.74	0.74
30	assign (segid 3A4 and resid 322 and name CA) (segid 3A4 and resid 345 and name CB)	6.21	0.90	0.89
	assign (segid 3A4 and resid 322 and name CA) (segid 3A4 and resid 345 and name N)	5.10	0.65	0.65
	assign (segid 3A4 and resid 322 and name CA) (segid 3A4 and resid 346 and name CA)	8.92	0.85	0.84
	assign (segid 3A4 and resid 322 and name CA) (segid 3A4 and resid 346 and name CB)	9.91	0.87	0.86
	assign (segid 3A4 and resid 322 and name CA) (segid 3A4 and resid 347 and name CA)	10.58	0.72	0.72
35	assign (segid 3A4 and resid 322 and name CA) (segid 3A4 and resid 347 and name CB)	10.34	0.61	0.62
	assign (segid 3A4 and resid 322 and name CA) (segid 3A4 and resid 348 and name CA)	13.37	0.73	0.72
	assign (segid 3A4 and resid 322 and name CA) (segid 3A4 and resid 349 and name CA)	14.25	0.76	0.76
	assign (segid 3A4 and resid 322 and name CA) (segid 3A4 and resid 349 and name CB)	13.64	0.76	0.76
	assign (segid 3A4 and resid 322 and name CA) (segid 3A4 and resid 350 and name CA)	14.52	0.78	0.77
40	assign (segid 3A4 and resid 322 and name CA) (segid 3A4 and resid 350 and name CB)	13.64	0.79	0.79
	assign (segid 3A4 and resid 322 and name CA) (segid 3A4 and resid 351 and name CA)	16.84	0.32	0.31
	assign (segid 3A4 and resid 322 and name CA) (segid 3A4 and resid 352 and name CA)	18.86	0.57	0.56
	assign (segid 3A4 and resid 322 and name CA) (segid 3A4 and resid 352 and name CB)	18.66	0.65	0.66
	assign (segid 3A4 and resid 322 and name CA) (segid 3A4 and resid 381 and name CA)	17.49	0.90	0.89
45	assign (segid 3A4 and resid 322 and name CA) (segid 3A4 and resid 382 and name CA)	13.95	0.77	0.76
	assign (segid 3A4 and resid 322 and name CA) (segid 3A4 and resid 382 and name CB)	12.97	0.89	0.89
	assign (segid 3A4 and resid 322 and name CA) (segid 3A4 and resid 383 and name CA)	14.09	0.50	0.50
	assign (segid 3A4 and resid 322 and name CA) (segid 3A4 and resid 384 and name CA)	13.71	0.47	0.46
	assign (segid 3A4 and resid 322 and name CA) (segid 3A4 and resid 384 and name CB)	15.01	0.48	0.49
50	assign (segid 3A4 and resid 322 and name CA) (segid 3A4 and resid 385 and name CA)	10.96	0.67	0.66
	assign (segid 3A4 and resid 322 and name CA) (segid 3A4 and resid 386 and name CA)	12.24	0.91	0.92
	assign (segid 3A4 and resid 322 and name CA) (segid 3A4 and resid 387 and name CA)	12.99	0.52	0.52
	assign (segid 3A4 and resid 322 and name CA) (segid 3A4 and resid 388 and name CA)	13.71	0.33	0.33
	assign (segid 3A4 and resid 322 and name CA) (segid 3A4 and resid 388 and name CB)	13.89	0.45	0.44
55	assign (segid 3A4 and resid 322 and name CA) (segid 3A4 and resid 389 and name CA)	11.28	0.46	0.46
	assign (segid 3A4 and resid 322 and name CA) (segid 3A4 and resid 389 and name CB)	9.87	0.43	0.43
	assign (segid 3A4 and resid 322 and name CA) (segid 3A4 and resid 390 and name CA)	12.89	0.66	0.66
	assign (segid 3A4 and resid 322 and name CA) (segid 3A4 and resid 390 and name CB)	14.05	0.67	0.67
	assign (segid 3A4 and resid 322 and name CA) (segid 3A4 and resid 391 and name CA)	14.18	0.52	0.51
60	assign (segid 3A4 and resid 322 and name CA) (segid 3A4 and resid 391 and name CB)	14.48	0.43	0.42
	assign (segid 3A4 and resid 322 and name CA) (segid 3A4 and resid 392 and name CA)	17.08	0.58	0.58
	assign (segid 3A4 and resid 322 and name CA) (segid 3A4 and resid 392 and name CB)	17.13	0.63	0.63
	assign (segid 3A4 and resid 322 and name CA) (segid 3A4 and resid 393 and name CA)	18.79	0.41	0.41
	assign (segid 3A4 and resid 322 and name CA) (segid 3A4 and resid 393 and name CB)	18.94	0.51	0.51
65	assign (segid 3A4 and resid 322 and name CA) (segid 3A4 and resid 394 and name CA)	18.48	0.54	0.54
	assign (segid 3A4 and resid 322 and name CA) (segid 3A4 and resid 430 and name CA)	13.37	2.21	2.21
	assign (segid 3A4 and resid 322 and name CA) (segid 3A4 and resid 431 and name CA)	11.32	2.09	2.08
	assign (segid 3A4 and resid 322 and name CA) (segid 3A4 and resid 433 and name CA)	16.15	0.92	0.93
	assign (segid 3A4 and resid 322 and name CA) (segid 3A4 and resid 322 and name C)	2.47	0.04	0.03
70	assign (segid 3A4 and resid 322 and name N) (segid 3A4 and resid 322 and name CA)	1.46	0.01	0.02
	assign (segid 3A4 and resid 322 and name N) (segid 3A4 and resid 322 and name O)	2.78	0.07	0.07
	assign (segid 3A4 and resid 322 and name N) (segid 3A4 and resid 323 and name C)	5.95	0.05	0.04
	assign (segid 3A4 and resid 322 and name N) (segid 3A4 and resid 323 and name CA)	4.86	0.04	0.04
	assign (segid 3A4 and resid 322 and name N) (segid 3A4 and resid 323 and name CB)	5.50	0.13	0.13
75	assign (segid 3A4 and resid 322 and name N) (segid 3A4 and resid 323 and name CG)	5.24	0.28	0.28
	assign (segid 3A4 and resid 322 and name N) (segid 3A4 and resid 323 and name N)	3.59	0.02	0.02
	assign (segid 3A4 and resid 322 and name N) (segid 3A4 and resid 323 and name O)	6.00	0.08	0.08
	assign (segid 3A4 and resid 322 and name N) (segid 3A4 and resid 324 and name N)	7.07	0.06	0.06
	assign (segid 3A4 and resid 322 and name N) (segid 3A4 and resid 343 and name C)	5.65	0.28	0.28
80	assign (segid 3A4 and resid 322 and name N) (segid 3A4 and resid 343 and name CA)	6.95	0.23	0.23
	assign (segid 3A4 and resid 322 and name N) (segid 3A4 and resid 343 and name N)	7.04	0.15	0.14
	assign (segid 3A4 and resid 322 and name N) (segid 3A4 and resid 343 and name O)	4.60	0.22	0.23

	assign (segid 3A4 and resid 322 and name N)	(segid 3A4 and resid 344 and name C)	5.79	0.54	0.55
	assign (segid 3A4 and resid 322 and name N)	(segid 3A4 and resid 344 and name CA)	5.24	0.37	0.36
	assign (segid 3A4 and resid 322 and name N)	(segid 3A4 and resid 344 and name CB)	5.92	0.23	0.22
	assign (segid 3A4 and resid 322 and name N)	(segid 3A4 and resid 344 and name N)	5.98	0.33	0.33
5	assign (segid 3A4 and resid 322 and name N)	(segid 3A4 and resid 345 and name N)	5.26	0.66	0.67
	assign (segid 3A4 and resid 322 and name N)	(segid HEM and resid 1 and name O1A)	6.61	0.68	0.67
	assign (segid 3A4 and resid 322 and name N)	(segid 3A4 and resid 323 and name C)	4.10	0.11	0.11
	assign (segid 3A4 and resid 322 and name O)	(segid 3A4 and resid 323 and name CA)	2.86	0.03	0.03
	assign (segid 3A4 and resid 322 and name O)	(segid 3A4 and resid 323 and name CB)	3.71	0.12	0.12
	assign (segid 3A4 and resid 322 and name O)	(segid 3A4 and resid 323 and name CG)	3.59	0.23	0.23
10	assign (segid 3A4 and resid 322 and name O)	(segid 3A4 and resid 323 and name N)	2.28	0.02	0.03
	assign (segid 3A4 and resid 322 and name O)	(segid 3A4 and resid 323 and name O)	4.64	0.15	0.15
	assign (segid 3A4 and resid 322 and name O)	(segid 3A4 and resid 324 and name C)	7.26	0.11	0.11
	assign (segid 3A4 and resid 322 and name O)	(segid 3A4 and resid 324 and name CA)	6.25	0.14	0.15
	assign (segid 3A4 and resid 322 and name O)	(segid 3A4 and resid 324 and name CB)	6.71	0.29	0.29
15	assign (segid 3A4 and resid 322 and name O)	(segid 3A4 and resid 324 and name N)	4.92	0.12	0.11
	assign (segid 3A4 and resid 322 and name O)	(segid 3A4 and resid 324 and name O)	7.25	0.11	0.12
	assign (segid 3A4 and resid 322 and name O)	(segid 3A4 and resid 342 and name C)	7.70	0.13	0.13
	assign (segid 3A4 and resid 322 and name O)	(segid 3A4 and resid 343 and name C)	6.04	0.09	0.10
	assign (segid 3A4 and resid 322 and name O)	(segid 3A4 and resid 343 and name CA)	6.91	0.06	0.06
20	assign (segid 3A4 and resid 322 and name O)	(segid 3A4 and resid 343 and name CB)	7.06	0.15	0.14
	assign (segid 3A4 and resid 322 and name O)	(segid 3A4 and resid 343 and name N)	6.66	0.08	0.07
	assign (segid 3A4 and resid 322 and name O)	(segid 3A4 and resid 343 and name O)	4.84	0.08	0.08
	assign (segid 3A4 and resid 322 and name O)	(segid 3A4 and resid 344 and name CA)	6.67	0.15	0.16
	assign (segid 3A4 and resid 322 and name O)	(segid 3A4 and resid 344 and name N)	6.88	0.12	0.12
25	assign (segid 3A4 and resid 322 and name O)	(segid 3A4 and resid 345 and name N)	6.81	0.48	0.48
	assign (segid 3A4 and resid 322 and name O)	(segid 3A4 and resid 323 and name CB)	2.48	0.03	0.03
	assign (segid 3A4 and resid 323 and name C)	(segid 3A4 and resid 323 and name CG)	3.89	0.04	0.04
	assign (segid 3A4 and resid 323 and name C)	(segid 3A4 and resid 323 and name O)	1.23	0.01	0.00
	assign (segid 3A4 and resid 323 and name C)	(segid 3A4 and resid 324 and name C)	3.49	0.07	0.08
30	assign (segid 3A4 and resid 323 and name C)	(segid 3A4 and resid 324 and name CA)	2.44	0.01	0.01
	assign (segid 3A4 and resid 323 and name C)	(segid 3A4 and resid 324 and name CB)	3.46	0.10	0.11
	assign (segid 3A4 and resid 323 and name C)	(segid 3A4 and resid 324 and name N)	1.34	0.01	0.01
	assign (segid 3A4 and resid 323 and name C)	(segid 3A4 and resid 324 and name O)	3.93	0.12	0.12
	assign (segid 3A4 and resid 323 and name C)	(segid 3A4 and resid 325 and name C)	6.58	0.06	0.06
35	assign (segid 3A4 and resid 323 and name C)	(segid 3A4 and resid 325 and name CA)	5.61	0.11	0.11
	assign (segid 3A4 and resid 323 and name C)	(segid 3A4 and resid 325 and name CB)	6.49	0.17	0.17
	assign (segid 3A4 and resid 323 and name C)	(segid 3A4 and resid 325 and name N)	4.36	0.10	0.10
	assign (segid 3A4 and resid 323 and name C)	(segid 3A4 and resid 325 and name O)	6.97	0.13	0.12
	assign (segid 3A4 and resid 323 and name C)	(segid 3A4 and resid 326 and name N)	7.24	0.21	0.20
40	assign (segid 3A4 and resid 323 and name C)	(segid 3A4 and resid 340 and name C)	7.40	0.29	0.29
	assign (segid 3A4 and resid 323 and name C)	(segid 3A4 and resid 341 and name C)	5.54	0.11	0.11
	assign (segid 3A4 and resid 323 and name C)	(segid 3A4 and resid 341 and name CA)	6.97	0.12	0.13
	assign (segid 3A4 and resid 323 and name C)	(segid 3A4 and resid 341 and name CB)	7.65	0.15	0.14
	assign (segid 3A4 and resid 323 and name C)	(segid 3A4 and resid 341 and name N)	7.24	0.14	0.14
45	assign (segid 3A4 and resid 323 and name C)	(segid 3A4 and resid 341 and name O)	4.68	0.12	0.13
	assign (segid 3A4 and resid 323 and name C)	(segid 3A4 and resid 342 and name C)	4.75	0.08	0.09
	assign (segid 3A4 and resid 323 and name C)	(segid 3A4 and resid 342 and name CA)	4.57	0.10	0.10
	assign (segid 3A4 and resid 323 and name C)	(segid 3A4 and resid 342 and name N)	5.57	0.12	0.11
	assign (segid 3A4 and resid 323 and name C)	(segid 3A4 and resid 342 and name O)	5.93	0.08	0.09
50	assign (segid 3A4 and resid 323 and name C)	(segid 3A4 and resid 343 and name C)	4.77	0.17	0.18
	assign (segid 3A4 and resid 323 and name C)	(segid 3A4 and resid 343 and name CA)	4.67	0.18	0.19
	assign (segid 3A4 and resid 323 and name C)	(segid 3A4 and resid 343 and name CB)	4.63	0.24	0.24
	assign (segid 3A4 and resid 323 and name C)	(segid 3A4 and resid 343 and name N)	3.91	0.13	0.14
	assign (segid 3A4 and resid 323 and name C)	(segid 3A4 and resid 343 and name O)	3.99	0.17	0.17
55	assign (segid 3A4 and resid 323 and name C)	(segid 3A4 and resid 344 and name C)	7.54	0.13	0.14
	assign (segid 3A4 and resid 323 and name C)	(segid 3A4 and resid 344 and name CA)	6.74	0.19	0.18
	assign (segid 3A4 and resid 323 and name C)	(segid 3A4 and resid 344 and name N)	6.07	0.18	0.17
	assign (segid 3A4 and resid 323 and name C)	(segid 3A4 and resid 345 and name N)	7.63	0.17	0.17
	assign (segid 3A4 and resid 323 and name C)	(segid 3A4 and resid 323 and name CB)	1.53	0.02	0.01
60	assign (segid 3A4 and resid 323 and name CA)	(segid 3A4 and resid 323 and name CB)	1.52	0.02	0.01
	assign (segid 3A4 and resid 323 and name CA)	(segid 3A4 and resid 323 and name CG)	2.60	0.02	0.02
	assign (segid 3A4 and resid 323 and name CA)	(segid 3A4 and resid 323 and name O)	2.40	0.02	0.01
	assign (segid 3A4 and resid 323 and name CA)	(segid 3A4 and resid 324 and name C)	4.67	0.09	0.08
	assign (segid 3A4 and resid 323 and name CA)	(segid 3A4 and resid 324 and name CA)	3.81	0.01	0.02
65	assign (segid 3A4 and resid 323 and name CA)	(segid 3A4 and resid 324 and name CB)	4.72	0.09	0.09
	assign (segid 3A4 and resid 323 and name CA)	(segid 3A4 and resid 324 and name N)	2.43	0.02	0.02
	assign (segid 3A4 and resid 323 and name CA)	(segid 3A4 and resid 324 and name O)	4.80	0.16	0.16
	assign (segid 3A4 and resid 323 and name CA)	(segid 3A4 and resid 325 and name C)	7.70	0.09	0.09
	assign (segid 3A4 and resid 323 and name CA)	(segid 3A4 and resid 325 and name CA)	6.72	0.12	0.12
70	assign (segid 3A4 and resid 323 and name CA)	(segid 3A4 and resid 325 and name CB)	7.64	0.18	0.17
	assign (segid 3A4 and resid 323 and name CA)	(segid 3A4 and resid 325 and name N)	5.61	0.09	0.10
	assign (segid 3A4 and resid 323 and name CA)	(segid 3A4 and resid 326 and name CA)	9.32	0.16	0.17
	assign (segid 3A4 and resid 323 and name CA)	(segid 3A4 and resid 326 and name CB)	9.59	0.14	0.13
	assign (segid 3A4 and resid 323 and name CA)	(segid 3A4 and resid 327 and name CA)	12.09	0.34	0.35
75	assign (segid 3A4 and resid 323 and name CA)	(segid 3A4 and resid 327 and name CB)	12.93	0.37	0.38
	assign (segid 3A4 and resid 323 and name CA)	(segid 3A4 and resid 328 and name CA)	13.42	0.41	0.41
	assign (segid 3A4 and resid 323 and name CA)	(segid 3A4 and resid 328 and name CB)	14.87	0.40	0.39
	assign (segid 3A4 and resid 323 and name CA)	(segid 3A4 and resid 329 and name CA)	12.93	0.65	0.64
	assign (segid 3A4 and resid 323 and name CA)	(segid 3A4 and resid 329 and name CB)	11.64	0.70	0.71
80	assign (segid 3A4 and resid 323 and name CA)	(segid 3A4 and resid 330 and name CA)	14.78	0.66	0.66
	assign (segid 3A4 and resid 323 and name CA)	(segid 3A4 and resid 330 and name CB)	16.28	0.66	0.66
	assign (segid 3A4 and resid 323 and name CA)	(segid 3A4 and resid 331 and name CA)	13.55	0.53	0.52

	assign (segid 3A4 and resid 323 and name CA) (segid 3A4 and resid 331 and name CB)	12.19	0.49	0.49
	assign (segid 3A4 and resid 323 and name CA) (segid 3A4 and resid 332 and name CA)	16.56	0.57	0.58
	assign (segid 3A4 and resid 323 and name CA) (segid 3A4 and resid 335 and name CA)	16.15	0.60	0.61
	assign (segid 3A4 and resid 323 and name CA) (segid 3A4 and resid 336 and name CA)	15.22	0.38	0.38
	assign (segid 3A4 and resid 323 and name CA) (segid 3A4 and resid 336 and name CB)	16.48	0.39	0.40
5	assign (segid 3A4 and resid 323 and name CA) (segid 3A4 and resid 337 and name CA)	11.90	0.39	0.40
	assign (segid 3A4 and resid 323 and name CA) (segid 3A4 and resid 337 and name CB)	10.62	0.40	0.40
	assign (segid 3A4 and resid 323 and name CA) (segid 3A4 and resid 338 and name CA)	12.67	0.27	0.27
	assign (segid 3A4 and resid 323 and name CA) (segid 3A4 and resid 338 and name CB)	13.53	0.27	0.27
	assign (segid 3A4 and resid 323 and name CA) (segid 3A4 and resid 339 and name CA)	11.42	0.18	0.18
10	assign (segid 3A4 and resid 323 and name CA) (segid 3A4 and resid 339 and name CB)	12.54	0.15	0.16
	assign (segid 3A4 and resid 323 and name CA) (segid 3A4 and resid 340 and name CA)	9.51	0.29	0.28
	assign (segid 3A4 and resid 323 and name CA) (segid 3A4 and resid 341 and name C)	6.98	0.11	0.12
	assign (segid 3A4 and resid 323 and name CA) (segid 3A4 and resid 341 and name CA)	8.44	0.13	0.13
	assign (segid 3A4 and resid 323 and name CA) (segid 3A4 and resid 341 and name CB)	9.03	0.18	0.17
15	assign (segid 3A4 and resid 323 and name CA) (segid 3A4 and resid 341 and name O)	6.15	0.14	0.14
	assign (segid 3A4 and resid 323 and name CA) (segid 3A4 and resid 342 and name C)	5.78	0.09	0.08
	assign (segid 3A4 and resid 323 and name CA) (segid 3A4 and resid 342 and name CA)	5.82	0.10	0.10
	assign (segid 3A4 and resid 323 and name CA) (segid 3A4 and resid 342 and name N)	6.93	0.11	0.12
	assign (segid 3A4 and resid 323 and name CA) (segid 3A4 and resid 342 and name O)	6.90	0.10	0.10
20	assign (segid 3A4 and resid 323 and name CA) (segid 3A4 and resid 343 and name C)	4.84	0.17	0.17
	assign (segid 3A4 and resid 323 and name CA) (segid 3A4 and resid 343 and name CA)	5.13	0.17	0.18
	assign (segid 3A4 and resid 323 and name CA) (segid 3A4 and resid 343 and name CB)	4.99	0.26	0.25
	assign (segid 3A4 and resid 323 and name CA) (segid 3A4 and resid 343 and name N)	4.73	0.12	0.12
	assign (segid 3A4 and resid 323 and name CA) (segid 3A4 and resid 343 and name O)	3.83	0.17	0.16
25	assign (segid 3A4 and resid 323 and name CA) (segid 3A4 and resid 344 and name C)	7.05	0.15	0.14
	assign (segid 3A4 and resid 323 and name CA) (segid 3A4 and resid 344 and name CA)	6.40	0.20	0.21
	assign (segid 3A4 and resid 323 and name CA) (segid 3A4 and resid 344 and name CB)	7.57	0.33	0.34
	assign (segid 3A4 and resid 323 and name CA) (segid 3A4 and resid 344 and name N)	6.01	0.18	0.19
	assign (segid 3A4 and resid 323 and name CA) (segid 3A4 and resid 344 and name O)	7.85	0.27	0.27
30	assign (segid 3A4 and resid 323 and name CA) (segid 3A4 and resid 345 and name CA)	7.40	0.43	0.43
	assign (segid 3A4 and resid 323 and name CA) (segid 3A4 and resid 345 and name CB)	6.89	0.20	0.19
	assign (segid 3A4 and resid 323 and name CA) (segid 3A4 and resid 345 and name N)	11.28	0.35	0.34
	assign (segid 3A4 and resid 323 and name CA) (segid 3A4 and resid 346 and name CA)	12.23	0.34	0.34
	assign (segid 3A4 and resid 323 and name CA) (segid 3A4 and resid 346 and name CB)	12.81	0.39	0.39
35	assign (segid 3A4 and resid 323 and name CA) (segid 3A4 and resid 347 and name CB)	12.67	0.39	0.40
	assign (segid 3A4 and resid 323 and name CA) (segid 3A4 and resid 348 and name CA)	16.00	0.42	0.43
	assign (segid 3A4 and resid 323 and name CA) (segid 3A4 and resid 349 and name CA)	16.39	0.31	0.31
	assign (segid 3A4 and resid 323 and name CA) (segid 3A4 and resid 349 and name CB)	15.68	0.29	0.28
	assign (segid 3A4 and resid 323 and name CA) (segid 3A4 and resid 350 and name CA)	16.08	0.41	0.42
40	assign (segid 3A4 and resid 323 and name CA) (segid 3A4 and resid 350 and name CB)	15.06	0.51	0.51
	assign (segid 3A4 and resid 323 and name CA) (segid 3A4 and resid 351 and name CA)	18.75	0.37	0.38
	assign (segid 3A4 and resid 323 and name CA) (segid 3A4 and resid 381 and name CA)	18.87	0.79	0.79
	assign (segid 3A4 and resid 323 and name CA) (segid 3A4 and resid 382 and name CA)	15.35	0.65	0.65
	assign (segid 3A4 and resid 323 and name CA) (segid 3A4 and resid 382 and name CB)	14.24	0.74	0.74
45	assign (segid 3A4 and resid 323 and name CA) (segid 3A4 and resid 383 and name CA)	16.20	0.63	0.62
	assign (segid 3A4 and resid 323 and name CA) (segid 3A4 and resid 384 and name CA)	15.39	0.69	0.69
	assign (segid 3A4 and resid 323 and name CA) (segid 3A4 and resid 384 and name CB)	16.54	0.74	0.74
	assign (segid 3A4 and resid 323 and name CA) (segid 3A4 and resid 385 and name CA)	12.14	0.73	0.73
50	assign (segid 3A4 and resid 323 and name CA) (segid 3A4 and resid 386 and name CA)	12.33	0.93	0.92
	assign (segid 3A4 and resid 323 and name CA) (segid 3A4 and resid 387 and name CA)	12.11	0.89	0.88
	assign (segid 3A4 and resid 323 and name CA) (segid 3A4 and resid 388 and name CA)	12.56	0.67	0.68
	assign (segid 3A4 and resid 323 and name CA) (segid 3A4 and resid 388 and name CB)	12.39	0.68	0.68
	assign (segid 3A4 and resid 323 and name CA) (segid 3A4 and resid 389 and name CA)	10.95	0.89	0.89
	assign (segid 3A4 and resid 323 and name CA) (segid 3A4 and resid 389 and name CB)	9.52	0.92	0.92
55	assign (segid 3A4 and resid 323 and name CA) (segid 3A4 and resid 390 and name CA)	13.27	0.98	0.99
	assign (segid 3A4 and resid 323 and name CA) (segid 3A4 and resid 390 and name CB)	14.29	0.96	0.95
	assign (segid 3A4 and resid 323 and name CA) (segid 3A4 and resid 391 and name CA)	15.30	0.86	0.87
	assign (segid 3A4 and resid 323 and name CA) (segid 3A4 and resid 391 and name CB)	15.91	0.76	0.76
	assign (segid 3A4 and resid 323 and name CA) (segid 3A4 and resid 392 and name CA)	17.89	0.93	0.92
60	assign (segid 3A4 and resid 323 and name CA) (segid 3A4 and resid 392 and name CB)	17.85	0.96	0.96
	assign (segid 3A4 and resid 323 and name CA) (segid 3A4 and resid 431 and name CA)	14.94	2.10	2.10
	assign (segid 3A4 and resid 323 and name CB) (segid 3A4 and resid 323 and name CG)	1.52	0.01	0.01
	assign (segid 3A4 and resid 323 and name CB) (segid 3A4 and resid 324 and name C)	4.84	0.16	0.16
	assign (segid 3A4 and resid 323 and name CB) (segid 3A4 and resid 324 and name CA)	4.42	0.09	0.08
65	assign (segid 3A4 and resid 323 and name CB) (segid 3A4 and resid 324 and name CB)	5.59	0.12	0.12
	assign (segid 3A4 and resid 323 and name CB) (segid 3A4 and resid 324 and name N)	3.10	0.10	0.11
	assign (segid 3A4 and resid 323 and name CB) (segid 3A4 and resid 324 and name O)	4.81	0.28	0.28
	assign (segid 3A4 and resid 323 and name CB) (segid 3A4 and resid 325 and name C)	7.62	0.20	0.19
	assign (segid 3A4 and resid 323 and name CB) (segid 3A4 and resid 325 and name CA)	6.52	0.22	0.21
70	assign (segid 3A4 and resid 323 and name CB) (segid 3A4 and resid 325 and name CB)	7.36	0.25	0.25
	assign (segid 3A4 and resid 323 and name CB) (segid 3A4 and resid 325 and name N)	5.66	0.17	0.16
	assign (segid 3A4 and resid 323 and name CB) (segid 3A4 and resid 326 and name CA)	9.20	0.27	0.27
	assign (segid 3A4 and resid 323 and name CB) (segid 3A4 and resid 326 and name CB)	9.38	0.26	0.26
	assign (segid 3A4 and resid 323 and name CB) (segid 3A4 and resid 327 and name CA)	11.77	0.49	0.49
75	assign (segid 3A4 and resid 323 and name CB) (segid 3A4 and resid 327 and name CB)	12.49	0.52	0.52
	assign (segid 3A4 and resid 323 and name CB) (segid 3A4 and resid 328 and name CA)	12.95	0.55	0.54
	assign (segid 3A4 and resid 323 and name CB) (segid 3A4 and resid 328 and name CB)	14.42	0.54	0.54
	assign (segid 3A4 and resid 323 and name CB) (segid 3A4 and resid 329 and name CA)	12.09	0.77	0.77
	assign (segid 3A4 and resid 323 and name CB) (segid 3A4 and resid 329 and name CB)	10.74	0.82	0.83
80	assign (segid 3A4 and resid 323 and name CB) (segid 3A4 and resid 330 and name CA)	13.81	0.16	0.16
	assign (segid 3A4 and resid 323 and name CB) (segid 3A4 and resid 330 and name CB)	15.30	0.77	0.77
	assign (segid 3A4 and resid 323 and name CB) (segid 3A4 and resid 331 and name CA)	12.43	0.57	0.57

	assign (segid 3A4 and resid 323 and name CB)	(segid 3A4 and resid 331 and name CB)	11.09	0.54	0.54
	assign (segid 3A4 and resid 323 and name CB)	(segid 3A4 and resid 332 and name CA)	15.42	0.62	0.62
	assign (segid 3A4 and resid 323 and name CB)	(segid 3A4 and resid 333 and name CA)	17.64	0.67	0.68
	assign (segid 3A4 and resid 323 and name CB)	(segid 3A4 and resid 335 and name CA)	15.38	0.64	0.64
	assign (segid 3A4 and resid 323 and name CB)	(segid 3A4 and resid 336 and name CA)	14.58	0.48	0.47
5	assign (segid 3A4 and resid 323 and name CB)	(segid 3A4 and resid 336 and name CB)	15.89	0.50	0.49
	assign (segid 3A4 and resid 323 and name CB)	(segid 3A4 and resid 337 and name CA)	11.45	0.49	0.48
	assign (segid 3A4 and resid 323 and name CB)	(segid 3A4 and resid 337 and name CB)	10.07	0.49	0.50
	assign (segid 3A4 and resid 323 and name CB)	(segid 3A4 and resid 338 and name CA)	12.54	0.35	0.35
	assign (segid 3A4 and resid 323 and name CB)	(segid 3A4 and resid 338 and name CB)	13.52	0.36	0.36
10	assign (segid 3A4 and resid 323 and name CB)	(segid 3A4 and resid 339 and name CA)	11.46	0.27	0.26
	assign (segid 3A4 and resid 323 and name CB)	(segid 3A4 and resid 339 and name CB)	12.60	0.26	0.26
	assign (segid 3A4 and resid 323 and name CB)	(segid 3A4 and resid 340 and name CA)	10.01	0.22	0.22
	assign (segid 3A4 and resid 323 and name CB)	(segid 3A4 and resid 341 and name C)	7.46	0.16	0.16
	assign (segid 3A4 and resid 323 and name CB)	(segid 3A4 and resid 341 and name CA)	8.85	0.18	0.18
	assign (segid 3A4 and resid 323 and name CB)	(segid 3A4 and resid 341 and name CB)	9.22	0.24	0.25
15	assign (segid 3A4 and resid 323 and name CB)	(segid 3A4 and resid 341 and name O)	6.53	0.18	0.18
	assign (segid 3A4 and resid 323 and name CB)	(segid 3A4 and resid 342 and name C)	6.25	0.20	0.20
	assign (segid 3A4 and resid 323 and name CB)	(segid 3A4 and resid 342 and name CA)	6.54	0.13	0.13
	assign (segid 3A4 and resid 323 and name CB)	(segid 3A4 and resid 342 and name N)	7.55	0.15	0.16
20	assign (segid 3A4 and resid 323 and name CB)	(segid 3A4 and resid 342 and name O)	7.25	0.23	0.23
	assign (segid 3A4 and resid 323 and name CB)	(segid 3A4 and resid 343 and name C)	4.95	0.35	0.35
	assign (segid 3A4 and resid 323 and name CB)	(segid 3A4 and resid 343 and name CA)	5.17	0.35	0.35
	assign (segid 3A4 and resid 323 and name CB)	(segid 3A4 and resid 343 and name CB)	4.60	0.45	0.44
	assign (segid 3A4 and resid 323 and name CB)	(segid 3A4 and resid 343 and name N)	5.09	0.25	0.26
25	assign (segid 3A4 and resid 323 and name CB)	(segid 3A4 and resid 343 and name O)	4.10	0.29	0.30
	assign (segid 3A4 and resid 323 and name CB)	(segid 3A4 and resid 344 and name C)	6.85	0.30	0.30
	assign (segid 3A4 and resid 323 and name CB)	(segid 3A4 and resid 344 and name CA)	6.50	0.41	0.40
	assign (segid 3A4 and resid 323 and name CB)	(segid 3A4 and resid 344 and name CB)	7.84	0.48	0.49
	assign (segid 3A4 and resid 323 and name CB)	(segid 3A4 and resid 344 and name N)	6.07	0.40	0.39
30	assign (segid 3A4 and resid 323 and name CB)	(segid 3A4 and resid 345 and name CA)	7.32	0.30	0.31
	assign (segid 3A4 and resid 323 and name CB)	(segid 3A4 and resid 345 and name CB)	6.69	0.36	0.37
	assign (segid 3A4 and resid 323 and name CB)	(segid 3A4 and resid 345 and name N)	6.58	0.31	0.30
	assign (segid 3A4 and resid 323 and name CB)	(segid 3A4 and resid 346 and name CA)	10.92	0.30	0.29
	assign (segid 3A4 and resid 323 and name CB)	(segid 3A4 and resid 346 and name CB)	11.90	0.29	0.30
35	assign (segid 3A4 and resid 323 and name CB)	(segid 3A4 and resid 347 and name CA)	12.29	0.42	0.42
	assign (segid 3A4 and resid 323 and name CB)	(segid 3A4 and resid 347 and name CB)	12.22	0.44	0.44
	assign (segid 3A4 and resid 323 and name CB)	(segid 3A4 and resid 348 and name CA)	15.63	0.42	0.42
	assign (segid 3A4 and resid 323 and name CB)	(segid 3A4 and resid 349 and name CA)	15.84	0.32	0.31
40	assign (segid 3A4 and resid 323 and name CB)	(segid 3A4 and resid 349 and name CB)	15.14	0.29	0.28
	assign (segid 3A4 and resid 323 and name CB)	(segid 3A4 and resid 350 and name CA)	15.24	0.47	0.48
	assign (segid 3A4 and resid 323 and name CB)	(segid 3A4 and resid 350 and name CB)	14.18	0.57	0.57
	assign (segid 3A4 and resid 323 and name CB)	(segid 3A4 and resid 351 and name CA)	18.01	0.53	0.53
	assign (segid 3A4 and resid 323 and name CB)	(segid 3A4 and resid 353 and name CB)	18.86	0.53	0.52
45	assign (segid 3A4 and resid 323 and name CB)	(segid 3A4 and resid 381 and name CA)	17.99	0.87	0.87
	assign (segid 3A4 and resid 323 and name CB)	(segid 3A4 and resid 382 and name CA)	14.55	0.72	0.73
	assign (segid 3A4 and resid 323 and name CB)	(segid 3A4 and resid 382 and name CB)	13.38	0.80	0.80
	assign (segid 3A4 and resid 323 and name CB)	(segid 3A4 and resid 383 and name CA)	15.71	0.74	0.74
	assign (segid 3A4 and resid 323 and name CB)	(segid 3A4 and resid 384 and name CA)	14.95	0.78	0.77
	assign (segid 3A4 and resid 323 and name CB)	(segid 3A4 and resid 384 and name CB)	16.07	0.81	0.80
50	assign (segid 3A4 and resid 323 and name CB)	(segid 3A4 and resid 385 and name CA)	11.52	0.78	0.78
	assign (segid 3A4 and resid 323 and name CB)	(segid 3A4 and resid 386 and name CA)	11.38	0.89	0.89
	assign (segid 3A4 and resid 323 and name CB)	(segid 3A4 and resid 387 and name CA)	11.10	0.92	0.93
	assign (segid 3A4 and resid 323 and name CB)	(segid 3A4 and resid 388 and name CA)	11.86	0.74	0.74
	assign (segid 3A4 and resid 323 and name CB)	(segid 3A4 and resid 388 and name CB)	11.71	0.78	0.77
55	assign (segid 3A4 and resid 323 and name CB)	(segid 3A4 and resid 389 and name CA)	10.56	0.90	0.91
	assign (segid 3A4 and resid 323 and name CB)	(segid 3A4 and resid 389 and name CB)	9.23	0.95	0.95
	assign (segid 3A4 and resid 323 and name CB)	(segid 3A4 and resid 390 and name CA)	12.74	1.00	1.00
	assign (segid 3A4 and resid 323 and name CB)	(segid 3A4 and resid 390 and name CB)	13.63	0.96	0.97
	assign (segid 3A4 and resid 323 and name CB)	(segid 3A4 and resid 391 and name CA)	15.06	0.91	0.91
60	assign (segid 3A4 and resid 323 and name CB)	(segid 3A4 and resid 391 and name CB)	15.67	0.81	0.81
	assign (segid 3A4 and resid 323 and name CB)	(segid 3A4 and resid 392 and name CA)	17.72	0.94	0.94
	assign (segid 3A4 and resid 323 and name CB)	(segid 3A4 and resid 392 and name CB)	17.78	0.96	0.95
	assign (segid 3A4 and resid 323 and name CB)	(segid 3A4 and resid 392 and name C)	6.17	0.14	0.13
65	assign (segid 3A4 and resid 323 and name CG)	(segid 3A4 and resid 324 and name CA)	5.83	0.10	0.10
	assign (segid 3A4 and resid 323 and name CG)	(segid 3A4 and resid 324 and name CB)	6.91	0.15	0.15
	assign (segid 3A4 and resid 323 and name CG)	(segid 3A4 and resid 324 and name N)	4.46	0.11	0.11
	assign (segid 3A4 and resid 323 and name CG)	(segid 3A4 and resid 324 and name O)	5.94	0.22	0.22
	assign (segid 3A4 and resid 323 and name CG)	(segid 3A4 and resid 325 and name N)	7.01	0.17	0.18
70	assign (segid 3A4 and resid 323 and name CG)	(segid 3A4 and resid 343 and name C)	5.74	0.29	0.29
	assign (segid 3A4 and resid 323 and name CG)	(segid 3A4 and resid 343 and name CA)	6.20	0.30	0.30
	assign (segid 3A4 and resid 323 and name CG)	(segid 3A4 and resid 343 and name CB)	5.56	0.41	0.41
	assign (segid 3A4 and resid 323 and name CG)	(segid 3A4 and resid 343 and name N)	6.35	0.22	0.22
	assign (segid 3A4 and resid 323 and name CG)	(segid 3A4 and resid 343 and name O)	4.84	0.21	0.21
75	assign (segid 3A4 and resid 323 and name CG)	(segid 3A4 and resid 344 and name C)	6.93	0.28	0.28
	assign (segid 3A4 and resid 323 and name CG)	(segid 3A4 and resid 344 and name CA)	6.82	0.36	0.37
	assign (segid 3A4 and resid 323 and name CG)	(segid 3A4 and resid 344 and name N)	6.67	0.36	0.35
	assign (segid 3A4 and resid 323 and name CG)	(segid 3A4 and resid 345 and name CA)	6.91	0.32	0.33
	assign (segid 3A4 and resid 323 and name CG)	(segid 3A4 and resid 345 and name CB)	6.05	0.38	0.37
80	assign (segid 3A4 and resid 323 and name CG)	(segid 3A4 and resid 345 and name N)	6.38	0.31	0.31
	assign (segid 3A4 and resid 323 and name CG)	(segid 3A4 and resid 323 and name C)	2.43	0.02	0.02
	assign (segid 3A4 and resid 323 and name N)	(segid 3A4 and resid 323 and name CA)	1.46	0.02	0.02
	assign (segid 3A4 and resid 323 and name N)	(segid 3A4 and resid 323 and name CB)	2.44	0.04	0.04

	assign (segid 3A4 and resid 324 and name C) (segid 3A4 and resid 341 and name CA)	5.71	0.12	0.12
	assign (segid 3A4 and resid 324 and name C) (segid 3A4 and resid 341 and name CB)	6.39	0.13	0.13
	assign (segid 3A4 and resid 324 and name C) (segid 3A4 and resid 341 and name CG)	7.62	0.18	0.19
	assign (segid 3A4 and resid 324 and name C) (segid 3A4 and resid 341 and name N)	5.30	0.13	0.14
	assign (segid 3A4 and resid 324 and name C) (segid 3A4 and resid 341 and name O)	3.60	0.08	0.08
5	assign (segid 3A4 and resid 324 and name C) (segid 3A4 and resid 342 and name C)	6.01	0.07	0.08
	assign (segid 3A4 and resid 324 and name C) (segid 3A4 and resid 342 and name CA)	5.46	0.09	0.08
	assign (segid 3A4 and resid 324 and name C) (segid 3A4 and resid 342 and name N)	5.59	0.09	0.09
	assign (segid 3A4 and resid 324 and name C) (segid 3A4 and resid 342 and name O)	6.99	0.10	0.10
	assign (segid 3A4 and resid 324 and name C) (segid 3A4 and resid 343 and name C)	7.37	0.18	0.17
10	assign (segid 3A4 and resid 324 and name C) (segid 3A4 and resid 343 and name CA)	6.61	0.22	0.21
	assign (segid 3A4 and resid 324 and name C) (segid 3A4 and resid 343 and name CB)	6.15	0.30	0.30
	assign (segid 3A4 and resid 324 and name C) (segid 3A4 and resid 343 and name N)	5.69	0.15	0.16
	assign (segid 3A4 and resid 324 and name C) (segid 3A4 and resid 343 and name O)	6.97	0.13	0.13
	assign (segid 3A4 and resid 324 and name CA) (segid 3A4 and resid 324 and name C)	1.52	0.00	0.01
15	assign (segid 3A4 and resid 324 and name CA) (segid 3A4 and resid 324 and name CB)	1.55	0.02	0.01
	assign (segid 3A4 and resid 324 and name CA) (segid 3A4 and resid 324 and name O)	2.39	0.01	0.00
	assign (segid 3A4 and resid 324 and name CA) (segid 3A4 and resid 325 and name C)	4.49	0.05	0.05
	assign (segid 3A4 and resid 324 and name CA) (segid 3A4 and resid 325 and name CA)	3.82	0.03	0.03
	assign (segid 3A4 and resid 324 and name CA) (segid 3A4 and resid 325 and name CB)	4.86	0.04	0.04
20	assign (segid 3A4 and resid 324 and name CA) (segid 3A4 and resid 325 and name N)	2.44	0.03	0.03
	assign (segid 3A4 and resid 324 and name CA) (segid 3A4 and resid 325 and name O)	4.69	0.19	0.19
	assign (segid 3A4 and resid 324 and name CA) (segid 3A4 and resid 326 and name C)	7.55	0.20	0.20
	assign (segid 3A4 and resid 324 and name CA) (segid 3A4 and resid 326 and name CA)	6.34	0.16	0.16
	assign (segid 3A4 and resid 324 and name CA) (segid 3A4 and resid 326 and name CB)	7.01	0.20	0.20
25	assign (segid 3A4 and resid 324 and name CA) (segid 3A4 and resid 326 and name N)	5.28	0.17	0.18
	assign (segid 3A4 and resid 324 and name CA) (segid 3A4 and resid 327 and name C)	9.07	0.20	0.21
	assign (segid 3A4 and resid 324 and name CA) (segid 3A4 and resid 327 and name CB)	10.14	0.20	0.19
	assign (segid 3A4 and resid 324 and name CA) (segid 3A4 and resid 328 and name C)	10.63	0.23	0.22
	assign (segid 3A4 and resid 324 and name CA) (segid 3A4 and resid 328 and name CB)	12.00	0.20	0.21
30	assign (segid 3A4 and resid 324 and name CA) (segid 3A4 and resid 329 and name C)	11.06	0.37	0.37
	assign (segid 3A4 and resid 324 and name CA) (segid 3A4 and resid 329 and name CB)	9.99	0.45	0.46
	assign (segid 3A4 and resid 324 and name CA) (segid 3A4 and resid 330 and name C)	13.53	0.34	0.35
	assign (segid 3A4 and resid 324 and name CA) (segid 3A4 and resid 330 and name CB)	14.97	0.32	0.31
	assign (segid 3A4 and resid 324 and name CA) (segid 3A4 and resid 331 and name C)	13.26	0.38	0.38
35	assign (segid 3A4 and resid 324 and name CA) (segid 3A4 and resid 331 and name CB)	12.05	0.30	0.31
	assign (segid 3A4 and resid 324 and name CA) (segid 3A4 and resid 332 and name C)	16.65	0.35	0.36
	assign (segid 3A4 and resid 324 and name CA) (segid 3A4 and resid 333 and name C)	18.07	0.34	0.33
	assign (segid 3A4 and resid 324 and name CA) (segid 3A4 and resid 333 and name CB)	15.22	0.40	0.39
	assign (segid 3A4 and resid 324 and name CA) (segid 3A4 and resid 335 and name C)	13.49	0.26	0.26
40	assign (segid 3A4 and resid 324 and name CA) (segid 3A4 and resid 336 and name C)	14.54	0.23	0.23
	assign (segid 3A4 and resid 324 and name CA) (segid 3A4 and resid 336 and name CB)	9.88	0.27	0.28
	assign (segid 3A4 and resid 324 and name CA) (segid 3A4 and resid 337 and name C)	8.88	0.29	0.28
	assign (segid 3A4 and resid 324 and name CA) (segid 3A4 and resid 337 and name CB)	9.69	0.32	0.32
	assign (segid 3A4 and resid 324 and name CA) (segid 3A4 and resid 338 and name C)	10.47	0.23	0.24
45	assign (segid 3A4 and resid 324 and name CA) (segid 3A4 and resid 338 and name CB)	7.36	0.31	0.31
	assign (segid 3A4 and resid 324 and name CA) (segid 3A4 and resid 339 and name C)	7.33	0.28	0.27
	assign (segid 3A4 and resid 324 and name CA) (segid 3A4 and resid 339 and name CB)	7.91	0.26	0.27
	assign (segid 3A4 and resid 324 and name CA) (segid 3A4 and resid 339 and name N)	8.98	0.23	0.23
50	assign (segid 3A4 and resid 324 and name CA) (segid 3A4 and resid 340 and name C)	5.43	0.35	0.35
	assign (segid 3A4 and resid 324 and name CA) (segid 3A4 and resid 340 and name CB)	5.80	0.34	0.34
	assign (segid 3A4 and resid 324 and name CA) (segid 3A4 and resid 340 and name N)	6.12	0.31	0.32
	assign (segid 3A4 and resid 324 and name CA) (segid 3A4 and resid 340 and name O)	5.57	0.47	0.48
	assign (segid 3A4 and resid 324 and name CA) (segid 3A4 and resid 341 and name C)	4.40	0.17	0.16
	assign (segid 3A4 and resid 324 and name CA) (segid 3A4 and resid 341 and name CB)	5.58	0.20	0.20
55	assign (segid 3A4 and resid 324 and name CA) (segid 3A4 and resid 341 and name N)	6.45	0.16	0.17
	assign (segid 3A4 and resid 324 and name CA) (segid 3A4 and resid 341 and name O)	5.43	0.23	0.23
	assign (segid 3A4 and resid 324 and name CA) (segid 3A4 and resid 342 and name C)	3.37	0.16	0.15
	assign (segid 3A4 and resid 324 and name CA) (segid 3A4 and resid 342 and name CB)	5.18	0.16	0.17
	assign (segid 3A4 and resid 324 and name CA) (segid 3A4 and resid 342 and name N)	4.49	0.14	0.14
60	assign (segid 3A4 and resid 324 and name CA) (segid 3A4 and resid 342 and name O)	4.90	0.18	0.17
	assign (segid 3A4 and resid 324 and name CA) (segid 3A4 and resid 343 and name C)	6.29	0.17	0.17
	assign (segid 3A4 and resid 324 and name CA) (segid 3A4 and resid 343 and name CB)	6.53	0.24	0.23
	assign (segid 3A4 and resid 324 and name CA) (segid 3A4 and resid 343 and name N)	5.93	0.28	0.28
	assign (segid 3A4 and resid 324 and name CA) (segid 3A4 and resid 343 and name O)	5.80	0.36	0.35
65	assign (segid 3A4 and resid 324 and name CA) (segid 3A4 and resid 343 and name N)	4.86	0.23	0.23
	assign (segid 3A4 and resid 324 and name CA) (segid 3A4 and resid 343 and name O)	6.03	0.20	0.20
	assign (segid 3A4 and resid 324 and name CA) (segid 3A4 and resid 344 and name C)	8.75	0.22	0.22
	assign (segid 3A4 and resid 324 and name CA) (segid 3A4 and resid 344 and name CB)	9.72	0.30	0.31
	assign (segid 3A4 and resid 324 and name CA) (segid 3A4 and resid 345 and name C)	10.86	0.21	0.21
70	assign (segid 3A4 and resid 324 and name CA) (segid 3A4 and resid 345 and name CB)	10.58	0.39	0.39
	assign (segid 3A4 and resid 324 and name CA) (segid 3A4 and resid 346 and name C)	14.36	0.27	0.27
	assign (segid 3A4 and resid 324 and name CA) (segid 3A4 and resid 346 and name CB)	15.10	0.24	0.24
	assign (segid 3A4 and resid 324 and name CA) (segid 3A4 and resid 347 and name C)	16.30	0.35	0.36
	assign (segid 3A4 and resid 324 and name CA) (segid 3A4 and resid 347 and name CB)	16.30	0.39	0.38
75	assign (segid 3A4 and resid 324 and name CA) (segid 3A4 and resid 349 and name C)	19.39	0.25	0.24
	assign (segid 3A4 and resid 324 and name CA) (segid 3A4 and resid 349 and name CB)	18.50	0.23	0.22
	assign (segid 3A4 and resid 324 and name CA) (segid 3A4 and resid 350 and name C)	19.16	0.34	0.35
	assign (segid 3A4 and resid 324 and name CA) (segid 3A4 and resid 350 and name CB)	18.21	0.45	0.46
	assign (segid 3A4 and resid 324 and name CA) (segid 3A4 and resid 382 and name C)	18.92	0.63	0.63
80	assign (segid 3A4 and resid 324 and name CA) (segid 3A4 and resid 382 and name CB)	17.74	0.71	0.70
	assign (segid 3A4 and resid 324 and name CA) (segid 3A4 and resid 384 and name C)	19.09	0.74	0.74
	assign (segid 3A4 and resid 324 and name CA) (segid 3A4 and resid 385 and name C)	15.76	0.77	0.77

	assign (segid 3A4 and resid 324 and name CA)	(segid 3A4 and resid 386 and name CA)	15.52	0.98	0.99
	assign (segid 3A4 and resid 324 and name CA)	(segid 3A4 and resid 387 and name CA)	14.74	1.10	1.09
	assign (segid 3A4 and resid 324 and name CA)	(segid 3A4 and resid 388 and name CA)	14.83	0.96	0.95
	assign (segid 3A4 and resid 324 and name CA)	(segid 3A4 and resid 388 and name CB)	14.31	0.95	0.95
5	assign (segid 3A4 and resid 324 and name CA)	(segid 3A4 and resid 389 and name CA)	13.73	1.10	1.11
	assign (segid 3A4 and resid 324 and name CA)	(segid 3A4 and resid 389 and name CB)	12.34	1.14	1.14
	assign (segid 3A4 and resid 324 and name CA)	(segid 3A4 and resid 390 and name CA)	16.50	1.11	1.11
	assign (segid 3A4 and resid 324 and name CA)	(segid 3A4 and resid 390 and name CB)	17.45	1.08	1.09
	assign (segid 3A4 and resid 324 and name CA)	(segid 3A4 and resid 391 and name CA)	18.68	0.95	0.96
10	assign (segid 3A4 and resid 324 and name CB)	(segid 3A4 and resid 325 and name C)	4.86	0.10	0.10
	assign (segid 3A4 and resid 324 and name CB)	(segid 3A4 and resid 325 and name CA)	4.65	0.08	0.08
	assign (segid 3A4 and resid 324 and name CB)	(segid 3A4 and resid 325 and name CB)	5.76	0.10	0.10
	assign (segid 3A4 and resid 324 and name CB)	(segid 3A4 and resid 325 and name N)	3.38	0.07	0.06
	assign (segid 3A4 and resid 324 and name CB)	(segid 3A4 and resid 325 and name O)	4.76	0.26	0.26
15	assign (segid 3A4 and resid 324 and name CB)	(segid 3A4 and resid 326 and name CA)	6.39	0.22	0.22
	assign (segid 3A4 and resid 324 and name CB)	(segid 3A4 and resid 326 and name CB)	7.05	0.27	0.28
	assign (segid 3A4 and resid 324 and name CB)	(segid 3A4 and resid 326 and name N)	5.62	0.22	0.23
	assign (segid 3A4 and resid 324 and name CB)	(segid 3A4 and resid 327 and name CA)	9.36	0.22	0.21
	assign (segid 3A4 and resid 324 and name CB)	(segid 3A4 and resid 327 and name CB)	10.46	0.18	0.18
20	assign (segid 3A4 and resid 324 and name CB)	(segid 3A4 and resid 328 and name CA)	11.23	0.26	0.26
	assign (segid 3A4 and resid 324 and name CB)	(segid 3A4 and resid 328 and name CB)	12.55	0.25	0.25
	assign (segid 3A4 and resid 324 and name CB)	(segid 3A4 and resid 329 and name CB)	12.08	0.34	0.35
	assign (segid 3A4 and resid 324 and name CB)	(segid 3A4 and resid 329 and name CB)	11.09	0.44	0.43
25	assign (segid 3A4 and resid 324 and name CB)	(segid 3A4 and resid 330 and name CA)	14.74	0.36	0.35
	assign (segid 3A4 and resid 324 and name CB)	(segid 3A4 and resid 330 and name CB)	16.14	0.32	0.33
	assign (segid 3A4 and resid 324 and name CB)	(segid 3A4 and resid 331 and name CA)	14.67	0.40	0.40
	assign (segid 3A4 and resid 324 and name CB)	(segid 3A4 and resid 331 and name CB)	13.50	0.34	0.33
	assign (segid 3A4 and resid 324 and name CB)	(segid 3A4 and resid 332 and name CA)	18.10	0.36	0.36
30	assign (segid 3A4 and resid 324 and name CB)	(segid 3A4 and resid 333 and name CA)	19.39	0.31	0.31
	assign (segid 3A4 and resid 324 and name CB)	(segid 3A4 and resid 335 and name CA)	16.45	0.40	0.40
	assign (segid 3A4 and resid 324 and name CB)	(segid 3A4 and resid 336 and name CA)	14.54	0.31	0.31
	assign (segid 3A4 and resid 324 and name CB)	(segid 3A4 and resid 336 and name CB)	15.50	0.27	0.27
	assign (segid 3A4 and resid 324 and name CB)	(segid 3A4 and resid 337 and name CA)	10.87	0.35	0.35
35	assign (segid 3A4 and resid 324 and name CB)	(segid 3A4 and resid 337 and name CB)	9.99	0.36	0.36
	assign (segid 3A4 and resid 324 and name CB)	(segid 3A4 and resid 338 and name CA)	10.19	0.45	0.45
	assign (segid 3A4 and resid 324 and name CB)	(segid 3A4 and resid 338 and name CB)	10.85	0.38	0.37
	assign (segid 3A4 and resid 324 and name CB)	(segid 3A4 and resid 339 and name CA)	8.02	0.43	0.43
	assign (segid 3A4 and resid 324 and name CB)	(segid 3A4 and resid 339 and name CB)	8.93	0.41	0.40
40	assign (segid 3A4 and resid 324 and name CB)	(segid 3A4 and resid 340 and name C)	5.19	0.53	0.53
	assign (segid 3A4 and resid 324 and name CB)	(segid 3A4 and resid 340 and name CA)	5.39	0.52	0.53
	assign (segid 3A4 and resid 324 and name CB)	(segid 3A4 and resid 340 and name N)	5.97	0.48	0.47
	assign (segid 3A4 and resid 324 and name CB)	(segid 3A4 and resid 340 and name O)	5.15	0.66	0.66
	assign (segid 3A4 and resid 324 and name CB)	(segid 3A4 and resid 341 and name C)	4.88	0.31	0.30
45	assign (segid 3A4 and resid 324 and name CB)	(segid 3A4 and resid 341 and name CA)	5.91	0.35	0.35
	assign (segid 3A4 and resid 324 and name CB)	(segid 3A4 and resid 341 and name CB)	7.04	0.31	0.30
	assign (segid 3A4 and resid 324 and name CB)	(segid 3A4 and resid 341 and name N)	5.57	0.39	0.38
	assign (segid 3A4 and resid 324 and name CB)	(segid 3A4 and resid 341 and name O)	4.06	0.26	0.26
	assign (segid 3A4 and resid 324 and name CB)	(segid 3A4 and resid 342 and name C)	6.04	0.29	0.28
50	assign (segid 3A4 and resid 324 and name CB)	(segid 3A4 and resid 342 and name CA)	5.02	0.28	0.27
	assign (segid 3A4 and resid 324 and name CB)	(segid 3A4 and resid 342 and name N)	5.32	0.31	0.31
	assign (segid 3A4 and resid 324 and name CB)	(segid 3A4 and resid 342 and name O)	7.15	0.29	0.28
	assign (segid 3A4 and resid 324 and name CB)	(segid 3A4 and resid 343 and name CA)	7.12	0.34	0.35
	assign (segid 3A4 and resid 324 and name CB)	(segid 3A4 and resid 343 and name CB)	7.18	0.39	0.40
55	assign (segid 3A4 and resid 324 and name CB)	(segid 3A4 and resid 343 and name N)	5.91	0.33	0.32
	assign (segid 3A4 and resid 324 and name CB)	(segid 3A4 and resid 343 and name O)	7.08	0.29	0.28
	assign (segid 3A4 and resid 324 and name CB)	(segid 3A4 and resid 344 and name CA)	9.76	0.28	0.29
	assign (segid 3A4 and resid 324 and name CB)	(segid 3A4 and resid 344 and name CB)	10.61	0.38	0.39
	assign (segid 3A4 and resid 324 and name CB)	(segid 3A4 and resid 345 and name CA)	12.07	0.26	0.26
60	assign (segid 3A4 and resid 324 and name CB)	(segid 3A4 and resid 345 and name CB)	11.81	0.42	0.43
	assign (segid 3A4 and resid 324 and name CB)	(segid 3A4 and resid 346 and name CA)	15.46	0.34	0.35
	assign (segid 3A4 and resid 324 and name CB)	(segid 3A4 and resid 346 and name CB)	16.21	0.30	0.31
	assign (segid 3A4 and resid 324 and name CB)	(segid 3A4 and resid 347 and name CA)	17.39	0.43	0.43
	assign (segid 3A4 and resid 324 and name CB)	(segid 3A4 and resid 347 and name CB)	17.31	0.46	0.45
65	assign (segid 3A4 and resid 324 and name CB)	(segid 3A4 and resid 382 and name CB)	18.89	0.71	0.70
	assign (segid 3A4 and resid 324 and name CB)	(segid 3A4 and resid 385 and name CA)	16.64	0.77	0.77
	assign (segid 3A4 and resid 324 and name CB)	(segid 3A4 and resid 386 and name CA)	16.51	0.99	1.00
	assign (segid 3A4 and resid 324 and name CB)	(segid 3A4 and resid 387 and name CA)	15.62	1.03	1.03
	assign (segid 3A4 and resid 324 and name CB)	(segid 3A4 and resid 388 and name CA)	15.39	0.87	0.86
	assign (segid 3A4 and resid 324 and name CB)	(segid 3A4 and resid 388 and name CB)	14.81	0.84	0.83
70	assign (segid 3A4 and resid 324 and name CB)	(segid 3A4 and resid 389 and name CA)	14.17	1.06	1.06
	assign (segid 3A4 and resid 324 and name CB)	(segid 3A4 and resid 389 and name CB)	12.76	1.09	1.09
	assign (segid 3A4 and resid 324 and name CB)	(segid 3A4 and resid 390 and name CA)	17.12	1.07	1.08
	assign (segid 3A4 and resid 324 and name CB)	(segid 3A4 and resid 390 and name CB)	18.15	1.05	1.04
75	assign (segid 3A4 and resid 324 and name N)	(segid 3A4 and resid 324 and name C)	2.40	0.05	0.04
	assign (segid 3A4 and resid 324 and name N)	(segid 3A4 and resid 324 and name CA)	1.47	0.02	0.01
	assign (segid 3A4 and resid 324 and name N)	(segid 3A4 and resid 324 and name CB)	2.50	0.03	0.04
	assign (segid 3A4 and resid 324 and name N)	(segid 3A4 and resid 324 and name O)	2.73	0.10	0.09
	assign (segid 3A4 and resid 324 and name N)	(segid 3A4 and resid 325 and name C)	5.50	0.07	0.07
	assign (segid 3A4 and resid 324 and name N)	(segid 3A4 and resid 325 and name CA)	4.71	0.05	0.05
80	assign (segid 3A4 and resid 324 and name N)	(segid 3A4 and resid 325 and name CB)	5.80	0.06	0.06
	assign (segid 3A4 and resid 324 and name N)	(segid 3A4 and resid 325 and name N)	3.49	0.04	0.04
	assign (segid 3A4 and resid 324 and name N)	(segid 3A4 and resid 325 and name O)	5.89	0.20	0.20
	assign (segid 3A4 and resid 324 and name N)	(segid 3A4 and resid 326 and name CA)	7.17	0.16	0.16

	assign (segid 3A4 and resid 324 and name N) (segid 3A4 and resid 326 and name CB)	7.60	0.14	0.15
	assign (segid 3A4 and resid 324 and name N) (segid 3A4 and resid 326 and name N)	6.09	0.18	0.17
	assign (segid 3A4 and resid 324 and name N) (segid 3A4 and resid 340 and name C)	6.85	0.34	0.33
	assign (segid 3A4 and resid 324 and name N) (segid 3A4 and resid 340 and name CA)	7.25	0.33	0.34
5	assign (segid 3A4 and resid 324 and name N) (segid 3A4 and resid 340 and name O)	6.93	0.48	0.49
	assign (segid 3A4 and resid 324 and name N) (segid 3A4 and resid 341 and name C)	5.48	0.14	0.14
	assign (segid 3A4 and resid 324 and name N) (segid 3A4 and resid 341 and name CA)	6.80	0.17	0.17
	assign (segid 3A4 and resid 324 and name N) (segid 3A4 and resid 341 and name CB)	7.55	0.13	0.13
	assign (segid 3A4 and resid 324 and name N) (segid 3A4 and resid 341 and name N)	6.79	0.20	0.20
10	assign (segid 3A4 and resid 324 and name N) (segid 3A4 and resid 341 and name O)	4.48	0.14	0.15
	assign (segid 3A4 and resid 324 and name N) (segid 3A4 and resid 342 and name C)	5.48	0.15	0.14
	assign (segid 3A4 and resid 324 and name N) (segid 3A4 and resid 342 and name CA)	5.05	0.13	0.12
	assign (segid 3A4 and resid 324 and name N) (segid 3A4 and resid 342 and name N)	5.78	0.15	0.15
	assign (segid 3A4 and resid 324 and name N) (segid 3A4 and resid 342 and name O)	6.64	0.15	0.14
15	assign (segid 3A4 and resid 324 and name N) (segid 3A4 and resid 343 and name C)	5.98	0.24	0.24
	assign (segid 3A4 and resid 324 and name N) (segid 3A4 and resid 343 and name CA)	5.68	0.27	0.28
	assign (segid 3A4 and resid 324 and name N) (segid 3A4 and resid 343 and name CB)	5.47	0.35	0.36
	assign (segid 3A4 and resid 324 and name N) (segid 3A4 and resid 343 and name N)	4.82	0.21	0.22
	assign (segid 3A4 and resid 324 and name N) (segid 3A4 and resid 343 and name O)	5.28	0.21	0.20
20	assign (segid 3A4 and resid 324 and name N) (segid 3A4 and resid 344 and name N)	7.29	0.24	0.24
	assign (segid 3A4 and resid 324 and name O) (segid 3A4 and resid 324 and name CB)	3.11	0.08	0.08
	assign (segid 3A4 and resid 324 and name O) (segid 3A4 and resid 325 and name C)	3.17	0.09	0.08
	assign (segid 3A4 and resid 324 and name O) (segid 3A4 and resid 325 and name CA)	2.76	0.03	0.03
	assign (segid 3A4 and resid 324 and name O) (segid 3A4 and resid 325 and name CB)	4.21	0.04	0.04
25	assign (segid 3A4 and resid 324 and name O) (segid 3A4 and resid 325 and name N)	2.24	0.02	0.02
	assign (segid 3A4 and resid 324 and name O) (segid 3A4 and resid 325 and name O)	3.84	0.26	0.25
	assign (segid 3A4 and resid 324 and name O) (segid 3A4 and resid 326 and name C)	5.87	0.16	0.16
	assign (segid 3A4 and resid 324 and name O) (segid 3A4 and resid 326 and name CA)	4.54	0.11	0.12
	assign (segid 3A4 and resid 324 and name O) (segid 3A4 and resid 326 and name CB)	4.94	0.18	0.17
30	assign (segid 3A4 and resid 324 and name O) (segid 3A4 and resid 326 and name N)	3.47	0.16	0.15
	assign (segid 3A4 and resid 324 and name O) (segid 3A4 and resid 326 and name O)	6.85	0.14	0.14
	assign (segid 3A4 and resid 324 and name O) (segid 3A4 and resid 327 and name CA)	7.53	0.25	0.25
	assign (segid 3A4 and resid 324 and name O) (segid 3A4 and resid 327 and name N)	6.16	0.24	0.23
	assign (segid 3A4 and resid 324 and name O) (segid 3A4 and resid 327 and name O)	6.94	0.31	0.30
35	assign (segid 3A4 and resid 324 and name O) (segid 3A4 and resid 338 and name O)	7.46	0.23	0.22
	assign (segid 3A4 and resid 324 and name O) (segid 3A4 and resid 339 and name C)	7.30	0.16	0.16
	assign (segid 3A4 and resid 324 and name O) (segid 3A4 and resid 339 and name CA)	7.48	0.19	0.18
	assign (segid 3A4 and resid 324 and name O) (segid 3A4 and resid 340 and name C)	6.43	0.24	0.24
	assign (segid 3A4 and resid 324 and name O) (segid 3A4 and resid 340 and name CA)	6.33	0.23	0.23
40	assign (segid 3A4 and resid 324 and name O) (segid 3A4 and resid 340 and name N)	6.18	0.19	0.19
	assign (segid 3A4 and resid 324 and name O) (segid 3A4 and resid 340 and name O)	6.93	0.36	0.36
	assign (segid 3A4 and resid 324 and name O) (segid 3A4 and resid 341 and name C)	5.98	0.08	0.08
	assign (segid 3A4 and resid 324 and name O) (segid 3A4 and resid 341 and name CA)	6.86	0.10	0.11
45	assign (segid 3A4 and resid 324 and name O) (segid 3A4 and resid 341 and name CB)	7.49	0.13	0.14
	assign (segid 3A4 and resid 324 and name O) (segid 3A4 and resid 341 and name N)	6.36	0.12	0.13
	assign (segid 3A4 and resid 324 and name O) (segid 3A4 and resid 341 and name O)	4.80	0.08	0.08
	assign (segid 3A4 and resid 324 and name O) (segid 3A4 and resid 342 and name C)	7.09	0.07	0.08
	assign (segid 3A4 and resid 324 and name O) (segid 3A4 and resid 342 and name CA)	6.60	0.11	0.10
50	assign (segid 3A4 and resid 324 and name O) (segid 3A4 and resid 342 and name N)	6.79	0.09	0.10
	assign (segid 3A4 and resid 324 and name O) (segid 3A4 and resid 343 and name CA)	7.44	0.15	0.15
	assign (segid 3A4 and resid 324 and name O) (segid 3A4 and resid 343 and name CB)	6.84	0.21	0.21
	assign (segid 3A4 and resid 324 and name O) (segid 3A4 and resid 343 and name N)	6.64	0.11	0.12
	assign (segid 3A4 and resid 324 and name O) (segid 3A4 and resid 343 and name O)	7.58	0.10	0.10
55	assign (segid 3A4 and resid 325 and name C) (segid 3A4 and resid 325 and name CB)	2.50	0.04	0.04
	assign (segid 3A4 and resid 325 and name C) (segid 3A4 and resid 325 and name O)	1.23	0.01	0.01
	assign (segid 3A4 and resid 325 and name C) (segid 3A4 and resid 326 and name C)	3.24	0.15	0.15
	assign (segid 3A4 and resid 325 and name C) (segid 3A4 and resid 326 and name CA)	2.46	0.02	0.02
	assign (segid 3A4 and resid 325 and name C) (segid 3A4 and resid 326 and name CB)	3.68	0.05	0.05
60	assign (segid 3A4 and resid 325 and name C) (segid 3A4 and resid 326 and name N)	1.33	0.01	0.01
	assign (segid 3A4 and resid 325 and name C) (segid 3A4 and resid 326 and name O)	4.27	0.20	0.20
	assign (segid 3A4 and resid 325 and name C) (segid 3A4 and resid 327 and name C)	4.83	0.20	0.20
	assign (segid 3A4 and resid 325 and name C) (segid 3A4 and resid 327 and name CA)	4.63	0.19	0.19
	assign (segid 3A4 and resid 325 and name C) (segid 3A4 and resid 327 and name CB)	5.73	0.12	0.12
65	assign (segid 3A4 and resid 325 and name C) (segid 3A4 and resid 327 and name N)	3.36	0.15	0.14
	assign (segid 3A4 and resid 325 and name C) (segid 3A4 and resid 327 and name O)	4.22	0.21	0.22
	assign (segid 3A4 and resid 325 and name C) (segid 3A4 and resid 328 and name C)	7.07	0.21	0.21
	assign (segid 3A4 and resid 325 and name C) (segid 3A4 and resid 328 and name CA)	6.75	0.21	0.20
	assign (segid 3A4 and resid 325 and name C) (segid 3A4 and resid 328 and name N)	6.02	0.19	0.20
	assign (segid 3A4 and resid 325 and name C) (segid 3A4 and resid 328 and name O)	7.40	0.27	0.27
70	assign (segid 3A4 and resid 325 and name C) (segid 3A4 and resid 329 and name CB)	7.10	0.27	0.27
	assign (segid 3A4 and resid 325 and name C) (segid 3A4 and resid 329 and name N)	7.31	0.22	0.22
	assign (segid 3A4 and resid 325 and name C) (segid 3A4 and resid 337 and name C)	7.42	0.12	0.13
	assign (segid 3A4 and resid 325 and name C) (segid 3A4 and resid 337 and name CB)	7.46	0.16	0.16
	assign (segid 3A4 and resid 325 and name C) (segid 3A4 and resid 337 and name O)	7.14	0.27	0.27
75	assign (segid 3A4 and resid 325 and name C) (segid 3A4 and resid 338 and name C)	5.78	0.20	0.21
	assign (segid 3A4 and resid 325 and name C) (segid 3A4 and resid 338 and name CA)	7.16	0.22	0.21
	assign (segid 3A4 and resid 325 and name C) (segid 3A4 and resid 338 and name N)	7.47	0.24	0.24
	assign (segid 3A4 and resid 325 and name C) (segid 3A4 and resid 338 and name O)	5.19	0.21	0.22
	assign (segid 3A4 and resid 325 and name C) (segid 3A4 and resid 339 and name C)	4.72	0.16	0.16
80	assign (segid 3A4 and resid 325 and name C) (segid 3A4 and resid 339 and name CA)	4.55	0.20	0.19
	assign (segid 3A4 and resid 325 and name C) (segid 3A4 and resid 339 and name CB)	5.30	0.16	0.17
	assign (segid 3A4 and resid 325 and name C) (segid 3A4 and resid 339 and name N)	5.55	0.21	0.21
	assign (segid 3A4 and resid 325 and name C) (segid 3A4 and resid 339 and name O)	5.90	0.15	0.16

	assign	(segid 3A4 and resid 325 and name C)	(segid 3A4 and resid 340 and name C)	5.21	0.12	0.12
	assign	(segid 3A4 and resid 325 and name C)	(segid 3A4 and resid 340 and name CA)	4.64	0.15	0.15
	assign	(segid 3A4 and resid 325 and name C)	(segid 3A4 and resid 340 and name N)	3.86	0.12	0.12
	assign	(segid 3A4 and resid 325 and name C)	(segid 3A4 and resid 340 and name O)	6.15	0.10	0.10
5	assign	(segid 3A4 and resid 325 and name C)	(segid 3A4 and resid 341 and name C)	5.86	0.14	0.15
	assign	(segid 3A4 and resid 325 and name C)	(segid 3A4 and resid 341 and name CA)	6.04	0.16	0.17
	assign	(segid 3A4 and resid 325 and name C)	(segid 3A4 and resid 341 and name CB)	6.48	0.19	0.18
	assign	(segid 3A4 and resid 325 and name C)	(segid 3A4 and resid 341 and name CG)	7.27	0.27	0.27
	assign	(segid 3A4 and resid 325 and name C)	(segid 3A4 and resid 341 and name N)	5.06	0.18	0.17
10	assign	(segid 3A4 and resid 325 and name C)	(segid 3A4 and resid 341 and name O)	4.88	0.14	0.15
	assign	(segid 3A4 and resid 325 and name C)	(segid 3A4 and resid 342 and name CA)	7.51	0.15	0.15
	assign	(segid 3A4 and resid 325 and name C)	(segid 3A4 and resid 342 and name N)	7.08	0.14	0.13
	assign	(segid 3A4 and resid 325 and name C)	(segid 3A4 and resid 325 and name C)	1.53	0.01	0.01
	assign	(segid 3A4 and resid 325 and name CA)	(segid 3A4 and resid 325 and name CB)	1.52	0.01	0.01
15	assign	(segid 3A4 and resid 325 and name CA)	(segid 3A4 and resid 325 and name O)	2.40	0.02	0.01
	assign	(segid 3A4 and resid 325 and name CA)	(segid 3A4 and resid 326 and name C)	4.58	0.13	0.13
	assign	(segid 3A4 and resid 325 and name CA)	(segid 3A4 and resid 326 and name CA)	3.82	0.02	0.03
	assign	(segid 3A4 and resid 325 and name CA)	(segid 3A4 and resid 326 and name CB)	4.84	0.05	0.04
	assign	(segid 3A4 and resid 325 and name CA)	(segid 3A4 and resid 326 and name N)	2.43	0.03	0.02
20	assign	(segid 3A4 and resid 325 and name CA)	(segid 3A4 and resid 326 and name O)	5.66	0.15	0.16
	assign	(segid 3A4 and resid 325 and name CA)	(segid 3A4 and resid 327 and name C)	5.40	0.26	0.25
	assign	(segid 3A4 and resid 325 and name CA)	(segid 3A4 and resid 327 and name CA)	5.57	0.24	0.23
	assign	(segid 3A4 and resid 325 and name CA)	(segid 3A4 and resid 327 and name CB)	6.61	0.17	0.18
	assign	(segid 3A4 and resid 325 and name CA)	(segid 3A4 and resid 327 and name N)	4.42	0.19	0.19
25	assign	(segid 3A4 and resid 325 and name CA)	(segid 3A4 and resid 327 and name O)	4.52	0.29	0.28
	assign	(segid 3A4 and resid 325 and name CA)	(segid 3A4 and resid 328 and name C)	7.09	0.24	0.25
	assign	(segid 3A4 and resid 325 and name CA)	(segid 3A4 and resid 328 and name CA)	6.96	0.24	0.24
	assign	(segid 3A4 and resid 325 and name CA)	(segid 3A4 and resid 328 and name CB)	8.40	0.23	0.23
	assign	(segid 3A4 and resid 325 and name CA)	(segid 3A4 and resid 328 and name N)	6.53	0.24	0.24
30	assign	(segid 3A4 and resid 325 and name CA)	(segid 3A4 and resid 329 and name CA)	7.54	0.29	0.28
	assign	(segid 3A4 and resid 325 and name CA)	(segid 3A4 and resid 329 and name CB)	6.57	0.34	0.33
	assign	(segid 3A4 and resid 325 and name CA)	(segid 3A4 and resid 329 and name N)	7.06	0.29	0.28
	assign	(segid 3A4 and resid 325 and name CA)	(segid 3A4 and resid 330 and name CA)	10.45	0.28	0.28
	assign	(segid 3A4 and resid 325 and name CA)	(segid 3A4 and resid 330 and name CB)	11.78	0.25	0.25
35	assign	(segid 3A4 and resid 325 and name CA)	(segid 3A4 and resid 331 and name CA)	10.95	0.36	0.35
	assign	(segid 3A4 and resid 325 and name CA)	(segid 3A4 and resid 331 and name CB)	10.04	0.32	0.31
	assign	(segid 3A4 and resid 325 and name CA)	(segid 3A4 and resid 332 and name CA)	14.58	0.36	0.36
	assign	(segid 3A4 and resid 325 and name CA)	(segid 3A4 and resid 333 and name CA)	15.60	0.43	0.43
	assign	(segid 3A4 and resid 325 and name CA)	(segid 3A4 and resid 335 and name CA)	13.01	0.34	0.34
40	assign	(segid 3A4 and resid 325 and name CA)	(segid 3A4 and resid 336 and name CA)	10.75	0.16	0.15
	assign	(segid 3A4 and resid 325 and name CA)	(segid 3A4 and resid 336 and name CB)	11.69	0.20	0.20
	assign	(segid 3A4 and resid 325 and name CA)	(segid 3A4 and resid 337 and name C)	6.88	0.19	0.18
	assign	(segid 3A4 and resid 325 and name CA)	(segid 3A4 and resid 337 and name CA)	7.37	0.20	0.21
	assign	(segid 3A4 and resid 325 and name CA)	(segid 3A4 and resid 337 and name CB)	6.47	0.19	0.19
45	assign	(segid 3A4 and resid 325 and name CA)	(segid 3A4 and resid 337 and name O)	6.73	0.29	0.29
	assign	(segid 3A4 and resid 325 and name CA)	(segid 3A4 and resid 338 and name C)	5.79	0.27	0.26
	assign	(segid 3A4 and resid 325 and name CA)	(segid 3A4 and resid 338 and name CA)	7.03	0.28	0.27
	assign	(segid 3A4 and resid 325 and name CA)	(segid 3A4 and resid 338 and name CB)	8.15	0.26	0.25
	assign	(segid 3A4 and resid 325 and name CA)	(segid 3A4 and resid 338 and name N)	7.04	0.30	0.31
50	assign	(segid 3A4 and resid 325 and name CA)	(segid 3A4 and resid 338 and name O)	5.00	0.30	0.31
	assign	(segid 3A4 and resid 325 and name CA)	(segid 3A4 and resid 339 and name C)	5.30	0.20	0.20
	assign	(segid 3A4 and resid 325 and name CA)	(segid 3A4 and resid 339 and name CA)	5.19	0.22	0.22
	assign	(segid 3A4 and resid 325 and name CA)	(segid 3A4 and resid 339 and name CB)	6.24	0.18	0.17
	assign	(segid 3A4 and resid 325 and name CA)	(segid 3A4 and resid 339 and name N)	5.89	0.25	0.26
55	assign	(segid 3A4 and resid 325 and name CA)	(segid 3A4 and resid 339 and name O)	6.39	0.22	0.21
	assign	(segid 3A4 and resid 325 and name CA)	(segid 3A4 and resid 340 and name C)	5.25	0.16	0.16
	assign	(segid 3A4 and resid 325 and name CA)	(segid 3A4 and resid 340 and name CA)	5.12	0.18	0.18
	assign	(segid 3A4 and resid 325 and name CA)	(segid 3A4 and resid 340 and name N)	4.47	0.17	0.18
	assign	(segid 3A4 and resid 325 and name CA)	(segid 3A4 and resid 340 and name O)	6.14	0.16	0.17
60	assign	(segid 3A4 and resid 325 and name CA)	(segid 3A4 and resid 341 and name C)	5.07	0.17	0.17
	assign	(segid 3A4 and resid 325 and name CA)	(segid 3A4 and resid 341 and name CA)	5.47	0.18	0.18
	assign	(segid 3A4 and resid 325 and name CA)	(segid 3A4 and resid 341 and name CB)	5.73	0.22	0.21
	assign	(segid 3A4 and resid 325 and name CA)	(segid 3A4 and resid 341 and name CG)	6.71	0.25	0.25
	assign	(segid 3A4 and resid 325 and name CA)	(segid 3A4 and resid 341 and name N)	4.80	0.19	0.20
65	assign	(segid 3A4 and resid 325 and name CA)	(segid 3A4 and resid 341 and name O)	3.99	0.16	0.15
	assign	(segid 3A4 and resid 325 and name CA)	(segid 3A4 and resid 342 and name C)	6.93	0.13	0.14
	assign	(segid 3A4 and resid 325 and name CA)	(segid 3A4 and resid 342 and name CA)	6.56	0.17	0.16
	assign	(segid 3A4 and resid 325 and name CA)	(segid 3A4 and resid 342 and name N)	6.23	0.16	0.16
	assign	(segid 3A4 and resid 325 and name CA)	(segid 3A4 and resid 342 and name O)	7.60	0.16	0.17
70	assign	(segid 3A4 and resid 325 and name CA)	(segid 3A4 and resid 343 and name CA)	7.52	0.25	0.25
	assign	(segid 3A4 and resid 325 and name CA)	(segid 3A4 and resid 343 and name CB)	6.80	0.33	0.33
	assign	(segid 3A4 and resid 325 and name CA)	(segid 3A4 and resid 343 and name N)	6.80	0.20	0.20
	assign	(segid 3A4 and resid 325 and name CA)	(segid 3A4 and resid 344 and name CA)	10.96	0.21	0.22
	assign	(segid 3A4 and resid 325 and name CA)	(segid 3A4 and resid 344 and name CB)	12.06	0.22	0.22
75	assign	(segid 3A4 and resid 325 and name CA)	(segid 3A4 and resid 345 and name CA)	12.56	0.28	0.28
	assign	(segid 3A4 and resid 325 and name CA)	(segid 3A4 and resid 345 and name CB)	12.17	0.41	0.42
	assign	(segid 3A4 and resid 325 and name CA)	(segid 3A4 and resid 346 and name CA)	16.23	0.27	0.26
	assign	(segid 3A4 and resid 325 and name CA)	(segid 3A4 and resid 346 and name CB)	16.86	0.22	0.23
	assign	(segid 3A4 and resid 325 and name CA)	(segid 3A4 and resid 347 and name CA)	18.14	0.31	0.30
80	assign	(segid 3A4 and resid 325 and name CA)	(segid 3A4 and resid 347 and name CB)	18.31	0.34	0.34
	assign	(segid 3A4 and resid 325 and name CA)	(segid 3A4 and resid 382 and name CB)	19.02	0.62	0.61
	assign	(segid 3A4 and resid 325 and name CA)	(segid 3A4 and resid 385 and name CA)	17.56	0.76	0.75
	assign	(segid 3A4 and resid 325 and name CA)	(segid 3A4 and resid 386 and name CA)	16.57	0.93	0.93

	assign	(segid 3A4 and resid 325 and name CA)	(segid 3A4 and resid 387 and name CA)	15.35	1.22	1.21
	assign	(segid 3A4 and resid 325 and name CA)	(segid 3A4 and resid 388 and name CA)	15.63	1.28	1.28
	assign	(segid 3A4 and resid 325 and name CA)	(segid 3A4 and resid 388 and name CB)	14.94	1.34	1.34
	assign	(segid 3A4 and resid 325 and name CA)	(segid 3A4 and resid 389 and name CA)	15.43	1.31	1.30
5	assign	(segid 3A4 and resid 325 and name CA)	(segid 3A4 and resid 389 and name CB)	14.22	1.32	1.32
	assign	(segid 3A4 and resid 325 and name CA)	(segid 3A4 and resid 390 and name CA)	18.17	1.25	1.24
	assign	(segid 3A4 and resid 325 and name CB)	(segid 3A4 and resid 326 and name C)	5.01	0.09	0.09
	assign	(segid 3A4 and resid 325 and name CB)	(segid 3A4 and resid 326 and name CA)	4.68	0.05	0.06
	assign	(segid 3A4 and resid 325 and name CB)	(segid 3A4 and resid 326 and name CB)	5.84	0.09	0.09
10	assign	(segid 3A4 and resid 325 and name CB)	(segid 3A4 and resid 326 and name N)	3.40	0.09	0.10
	assign	(segid 3A4 and resid 325 and name CB)	(segid 3A4 and resid 326 and name O)	6.06	0.14	0.15
	assign	(segid 3A4 and resid 325 and name CB)	(segid 3A4 and resid 327 and name C)	4.79	0.22	0.21
	assign	(segid 3A4 and resid 325 and name CB)	(segid 3A4 and resid 327 and name CA)	5.35	0.20	0.20
	assign	(segid 3A4 and resid 325 and name CB)	(segid 3A4 and resid 327 and name CB)	6.49	0.10	0.10
15	assign	(segid 3A4 and resid 325 and name CB)	(segid 3A4 and resid 327 and name N)	4.52	0.12	0.13
	assign	(segid 3A4 and resid 325 and name CB)	(segid 3A4 and resid 327 and name O)	3.79	0.22	0.23
	assign	(segid 3A4 and resid 325 and name CB)	(segid 3A4 and resid 328 and name C)	6.06	0.21	0.22
	assign	(segid 3A4 and resid 325 and name CB)	(segid 3A4 and resid 328 and name CA)	5.91	0.22	0.22
	assign	(segid 3A4 and resid 325 and name CB)	(segid 3A4 and resid 328 and name CB)	7.31	0.21	0.21
20	assign	(segid 3A4 and resid 325 and name CB)	(segid 3A4 and resid 328 and name N)	5.74	0.22	0.21
	assign	(segid 3A4 and resid 325 and name CB)	(segid 3A4 and resid 328 and name O)	6.68	0.27	0.27
	assign	(segid 3A4 and resid 325 and name CB)	(segid 3A4 and resid 329 and name C)	7.17	0.22	0.22
	assign	(segid 3A4 and resid 325 and name CB)	(segid 3A4 and resid 329 and name CA)	6.45	0.26	0.27
	assign	(segid 3A4 and resid 325 and name CB)	(segid 3A4 and resid 329 and name CB)	5.64	0.34	0.35
25	assign	(segid 3A4 and resid 325 and name CB)	(segid 3A4 and resid 329 and name N)	5.89	0.26	0.25
	assign	(segid 3A4 and resid 325 and name CB)	(segid 3A4 and resid 329 and name O)	6.94	0.25	0.26
	assign	(segid 3A4 and resid 325 and name CB)	(segid 3A4 and resid 330 and name C)	9.25	0.25	0.24
	assign	(segid 3A4 and resid 325 and name CB)	(segid 3A4 and resid 330 and name CB)	10.58	0.21	0.22
	assign	(segid 3A4 and resid 325 and name CB)	(segid 3A4 and resid 331 and name CA)	9.93	0.37	0.38
30	assign	(segid 3A4 and resid 325 and name CB)	(segid 3A4 and resid 331 and name CB)	9.08	0.35	0.36
	assign	(segid 3A4 and resid 325 and name CB)	(segid 3A4 and resid 332 and name CA)	13.55	0.31	0.32
	assign	(segid 3A4 and resid 325 and name CB)	(segid 3A4 and resid 333 and name CA)	14.36	0.32	0.33
	assign	(segid 3A4 and resid 325 and name CB)	(segid 3A4 and resid 335 and name CA)	11.64	0.30	0.29
	assign	(segid 3A4 and resid 325 and name CB)	(segid 3A4 and resid 336 and name CA)	9.28	0.15	0.15
35	assign	(segid 3A4 and resid 325 and name CB)	(segid 3A4 and resid 336 and name CB)	10.21	0.19	0.19
	assign	(segid 3A4 and resid 325 and name CB)	(segid 3A4 and resid 337 and name C)	5.39	0.21	0.20
	assign	(segid 3A4 and resid 325 and name CB)	(segid 3A4 and resid 337 and name CA)	5.89	0.21	0.20
	assign	(segid 3A4 and resid 325 and name CB)	(segid 3A4 and resid 337 and name CB)	5.06	0.17	0.17
	assign	(segid 3A4 and resid 325 and name CB)	(segid 3A4 and resid 337 and name N)	6.99	0.17	0.16
40	assign	(segid 3A4 and resid 325 and name CB)	(segid 3A4 and resid 337 and name O)	5.27	0.30	0.31
	assign	(segid 3A4 and resid 325 and name CB)	(segid 3A4 and resid 338 and name C)	4.59	0.33	0.33
	assign	(segid 3A4 and resid 325 and name CB)	(segid 3A4 and resid 338 and name CA)	5.69	0.32	0.32
	assign	(segid 3A4 and resid 325 and name CB)	(segid 3A4 and resid 338 and name CB)	6.88	0.32	0.31
	assign	(segid 3A4 and resid 325 and name CB)	(segid 3A4 and resid 338 and name N)	5.59	0.33	0.34
45	assign	(segid 3A4 and resid 325 and name CB)	(segid 3A4 and resid 338 and name O)	3.82	0.40	0.41
	assign	(segid 3A4 and resid 325 and name CB)	(segid 3A4 and resid 339 and name C)	4.80	0.30	0.29
	assign	(segid 3A4 and resid 325 and name CB)	(segid 3A4 and resid 339 and name CA)	4.53	0.27	0.27
	assign	(segid 3A4 and resid 325 and name CB)	(segid 3A4 and resid 339 and name CB)	5		

	assign (segid 3A4 and resid 325 and name N)	(segid 3A4 and resid 325 and name CA)	1.47	0.02	0.01
	assign (segid 3A4 and resid 325 and name N)	(segid 3A4 and resid 325 and name CB)	2.45	0.02	0.02
	assign (segid 3A4 and resid 325 and name N)	(segid 3A4 and resid 325 and name O)	2.91	0.09	0.09
	assign (segid 3A4 and resid 325 and name N)	(segid 3A4 and resid 326 and name C)	5.71	0.17	0.16
	assign (segid 3A4 and resid 325 and name N)	(segid 3A4 and resid 326 and name CA)	4.77	0.09	0.08
5	assign (segid 3A4 and resid 325 and name N)	(segid 3A4 and resid 326 and name CB)	5.73	0.11	0.10
	assign (segid 3A4 and resid 325 and name N)	(segid 3A4 and resid 326 and name N)	3.49	0.10	0.09
	assign (segid 3A4 and resid 325 and name N)	(segid 3A4 and resid 326 and name O)	6.71	0.22	0.22
	assign (segid 3A4 and resid 325 and name N)	(segid 3A4 and resid 327 and name C)	6.73	0.20	0.21
	assign (segid 3A4 and resid 325 and name N)	(segid 3A4 and resid 327 and name CA)	6.88	0.19	0.20
10	assign (segid 3A4 and resid 325 and name N)	(segid 3A4 and resid 327 and name N)	5.70	0.15	0.16
	assign (segid 3A4 and resid 325 and name N)	(segid 3A4 and resid 327 and name O)	5.85	0.20	0.21
	assign (segid 3A4 and resid 325 and name N)	(segid 3A4 and resid 327 and name C)	7.55	0.22	0.22
	assign (segid 3A4 and resid 325 and name N)	(segid 3A4 and resid 327 and name CB)	6.97	0.23	0.24
	assign (segid 3A4 and resid 325 and name N)	(segid 3A4 and resid 327 and name O)	6.37	0.28	0.29
15	assign (segid 3A4 and resid 325 and name N)	(segid 3A4 and resid 328 and name C)	5.40	0.30	0.30
	assign (segid 3A4 and resid 325 and name N)	(segid 3A4 and resid 328 and name CA)	5.64	0.21	0.20
	assign (segid 3A4 and resid 325 and name N)	(segid 3A4 and resid 328 and name CB)	5.90	0.23	0.22
	assign (segid 3A4 and resid 325 and name N)	(segid 3A4 and resid 328 and name N)	7.03	0.18	0.18
	assign (segid 3A4 and resid 325 and name N)	(segid 3A4 and resid 328 and name O)	6.62	0.26	0.27
20	assign (segid 3A4 and resid 325 and name N)	(segid 3A4 and resid 329 and name C)	6.59	0.21	0.21
	assign (segid 3A4 and resid 325 and name N)	(segid 3A4 and resid 329 and name CA)	4.69	0.18	0.19
	assign (segid 3A4 and resid 325 and name N)	(segid 3A4 and resid 329 and name CB)	4.84	0.20	0.20
	assign (segid 3A4 and resid 325 and name N)	(segid 3A4 and resid 329 and name N)	4.61	0.22	0.22
	assign (segid 3A4 and resid 325 and name N)	(segid 3A4 and resid 329 and name O)	5.36	0.24	0.24
25	assign (segid 3A4 and resid 325 and name N)	(segid 3A4 and resid 341 and name C)	4.10	0.11	0.10
	assign (segid 3A4 and resid 325 and name N)	(segid 3A4 and resid 341 and name CA)	4.81	0.10	0.11
	assign (segid 3A4 and resid 325 and name N)	(segid 3A4 and resid 341 and name CB)	5.33	0.14	0.13
	assign (segid 3A4 and resid 325 and name N)	(segid 3A4 and resid 341 and name N)	6.50	0.17	0.17
	assign (segid 3A4 and resid 325 and name N)	(segid 3A4 and resid 341 and name O)	4.35	0.14	0.13
30	assign (segid 3A4 and resid 325 and name N)	(segid 3A4 and resid 341 and name C)	2.93	0.11	0.10
	assign (segid 3A4 and resid 325 and name N)	(segid 3A4 and resid 342 and name CA)	5.78	0.10	0.10
	assign (segid 3A4 and resid 325 and name N)	(segid 3A4 and resid 342 and name N)	5.29	0.13	0.13
	assign (segid 3A4 and resid 325 and name N)	(segid 3A4 and resid 342 and name O)	5.13	0.11	0.11
	assign (segid 3A4 and resid 325 and name N)	(segid 3A4 and resid 342 and name C)	6.59	0.12	0.13
35	assign (segid 3A4 and resid 325 and name N)	(segid 3A4 and resid 343 and name CA)	7.52	0.21	0.21
	assign (segid 3A4 and resid 325 and name N)	(segid 3A4 and resid 343 and name CB)	6.52	0.25	0.26
	assign (segid 3A4 and resid 325 and name N)	(segid 3A4 and resid 343 and name N)	6.02	0.35	0.34
	assign (segid 3A4 and resid 325 and name N)	(segid 3A4 and resid 343 and name O)	5.65	0.19	0.19
	assign (segid 3A4 and resid 325 and name N)	(segid 3A4 and resid 343 and name C)	7.33	0.16	0.16
40	assign (segid 3A4 and resid 325 and name N)	(segid 3A4 and resid 325 and name CB)	3.04	0.13	0.13
	assign (segid 3A4 and resid 325 and name O)	(segid 3A4 and resid 326 and name C)	3.39	0.24	0.23
	assign (segid 3A4 and resid 325 and name O)	(segid 3A4 and resid 326 and name CA)	2.81	0.04	0.04
	assign (segid 3A4 and resid 325 and name O)	(segid 3A4 and resid 326 and name CB)	4.21	0.08	0.07
	assign (segid 3A4 and resid 325 and name O)	(segid 3A4 and resid 326 and name N)	2.25	0.02	0.02
45	assign (segid 3A4 and resid 325 and name O)	(segid 3A4 and resid 326 and name O)	4.18	0.38	0.38
	assign (segid 3A4 and resid 325 and name O)	(segid 3A4 and resid 326 and name C)	5.02	0.29	0.29
	assign (segid 3A4 and resid 325 and name O)	(segid 3A4 and resid 327 and name CA)	4.77	0.23	0.23
	assign (segid 3A4 and resid 325 and name O)	(segid 3A4 and resid 327 and name CB)	6.03	0.18	0.17
	assign (segid 3A4 and resid 325 and name O)	(segid 3A4 and resid 327 and name N)	3.63	0.16	0.16
50	assign (segid 3A4 and resid 325 and name O)	(segid 3A4 and resid 327 and name O)	4.57	0.31	0.31
	assign (segid 3A4 and resid 325 and name O)	(segid 3A4 and resid 328 and name C)	7.44	0.32	0.32
	assign (segid 3A4 and resid 325 and name O)	(segid 3A4 and resid 328 and name CA)	6.88	0.34	0.34
	assign (segid 3A4 and resid 325 and name O)	(segid 3A4 and resid 328 and name N)	6.12	0.31	0.32
	assign (segid 3A4 and resid 325 and name O)	(segid 3A4 and resid 328 and name O)	7.47	0.13	0.12
55	assign (segid 3A4 and resid 325 and name O)	(segid 3A4 and resid 337 and name C)	7.26	0.30	0.30
	assign (segid 3A4 and resid 325 and name O)	(segid 3A4 and resid 337 and name CA)	5.35	0.18	0.18
	assign (segid 3A4 and resid 325 and name O)	(segid 3A4 and resid 338 and name N)	6.82	0.18	0.18
	assign (segid 3A4 and resid 325 and name O)	(segid 3A4 and resid 338 and name O)	7.31	0.21	0.20
60	assign (segid 3A4 and resid 325 and name O)	(segid 3A4 and resid 338 and name C)	4.78	0.19	0.19
	assign (segid 3A4 and resid 325 and name O)	(segid 3A4 and resid 339 and name CA)	3.77	0.16	0.16
	assign (segid 3A4 and resid 325 and name O)	(segid 3A4 and resid 339 and name N)	3.85	0.18	0.18
	assign (segid 3A4 and resid 325 and name O)	(segid 3A4 and resid 339 and name CB)	4.57	0.15	0.14
	assign (segid 3A4 and resid 325 and name O)	(segid 3A4 and resid 339 and name O)	5.02	0.18	0.18
	assign (segid 3A4 and resid 325 and name O)	(segid 3A4 and resid 339 and name C)	4.93	0.16	0.16
65	assign (segid 3A4 and resid 325 and name O)	(segid 3A4 and resid 340 and name CA)	4.31	0.11	0.12
	assign (segid 3A4 and resid 325 and name O)	(segid 3A4 and resid 340 and name N)	3.54	0.15	0.14
	assign (segid 3A4 and resid 325 and name O)	(segid 3A4 and resid 340 and name O)	2.80	0.14	0.14
	assign (segid 3A4 and resid 325 and name O)	(segid 3A4 and resid 340 and name C)	5.27	0.08	0.08
	assign (segid 3A4 and resid 325 and name O)	(segid 3A4 and resid 341 and name C)	5.55	0.13	0.13
70	assign (segid 3A4 and resid 325 and name O)	(segid 3A4 and resid 341 and name CA)	5.55	0.17	0.17
	assign (segid 3A4 and resid 325 and name O)	(segid 3A4 and resid 341 and name CB)	6.15	0.20	0.19
	assign (segid 3A4 and resid 325 and name O)	(segid 3A4 and resid 341 and name N)	6.83	0.29	0.30
	assign (segid 3A4 and resid 325 and name O)	(segid 3A4 and resid 341 and name O)	4.38	0.19	0.18
	assign (segid 3A4 and resid 325 and name O)	(segid 3A4 and resid 341 and name C)	4.74	0.13	0.12
75	assign (segid 3A4 and resid 325 and name O)	(segid 3A4 and resid 342 and name CA)	7.37	0.15	0.14
	assign (segid 3A4 and resid 325 and name O)	(segid 3A4 and resid 342 and name N)	6.78	0.13	0.12
	assign (segid 3A4 and resid 325 and name O)	(segid 3A4 and resid 342 and name O)	2.48	0.02	0.03
	assign (segid 3A4 and resid 326 and name C)	(segid 3A4 and resid 326 and name CB)	1.23	0.01	0.01
	assign (segid 3A4 and resid 326 and name C)	(segid 3A4 and resid 327 and name C)	3.61	0.06	0.05
80	assign (segid 3A4 and resid 326 and name C)	(segid 3A4 and resid 327 and name CA)	2.46	0.02	0.01
	assign (segid 3A4 and resid 326 and name C)	(segid 3A4 and resid 327 and name CB)	3.19	0.15	0.14
	assign (segid 3A4 and resid 326 and name C)	(segid 3A4 and resid 327 and name N)	1.32	0.01	0.02

	assign	(segid 3A4 and resid 326 and name C)	(segid 3A4 and resid 327 and name O)	3.85	0.07	0.08
	assign	(segid 3A4 and resid 326 and name C)	(segid 3A4 and resid 328 and name C)	6.41	0.15	0.15
	assign	(segid 3A4 and resid 326 and name C)	(segid 3A4 and resid 328 and name CA)	5.98	0.12	0.11
	assign	(segid 3A4 and resid 326 and name C)	(segid 3A4 and resid 328 and name CB)	7.14	0.09	0.09
5	assign	(segid 3A4 and resid 326 and name C)	(segid 3A4 and resid 328 and name N)	4.72	0.08	0.07
	assign	(segid 3A4 and resid 326 and name C)	(segid 3A4 and resid 328 and name O)	6.34	0.28	0.29
	assign	(segid 3A4 and resid 326 and name C)	(segid 3A4 and resid 329 and name CB)	7.38	0.16	0.16
	assign	(segid 3A4 and resid 326 and name C)	(segid 3A4 and resid 329 and name N)	7.19	0.07	0.08
	assign	(segid 3A4 and resid 326 and name C)	(segid 3A4 and resid 329 and name O)	6.63	0.20	0.20
10	assign	(segid 3A4 and resid 326 and name C)	(segid 3A4 and resid 338 and name C)	6.63	0.16	0.17
	assign	(segid 3A4 and resid 326 and name C)	(segid 3A4 and resid 338 and name O)	5.49	0.14	0.13
	assign	(segid 3A4 and resid 326 and name C)	(segid 3A4 and resid 339 and name C)	4.70	0.19	0.19
	assign	(segid 3A4 and resid 326 and name C)	(segid 3A4 and resid 339 and name CA)	4.50	0.19	0.20
	assign	(segid 3A4 and resid 326 and name C)	(segid 3A4 and resid 339 and name CB)	5.80	0.25	0.24
	assign	(segid 3A4 and resid 326 and name C)	(segid 3A4 and resid 339 and name N)	6.65	0.14	0.14
15	assign	(segid 3A4 and resid 326 and name C)	(segid 3A4 and resid 339 and name O)	7.36	0.24	0.23
	assign	(segid 3A4 and resid 326 and name C)	(segid 3A4 and resid 340 and name C)	6.26	0.29	0.29
	assign	(segid 3A4 and resid 326 and name C)	(segid 3A4 and resid 340 and name CA)	5.16	0.20	0.20
	assign	(segid 3A4 and resid 326 and name C)	(segid 3A4 and resid 340 and name N)	7.37	0.23	0.23
20	assign	(segid 3A4 and resid 326 and name C)	(segid 3A4 and resid 341 and name N)	1.53	0.00	0.00
	assign	(segid 3A4 and resid 326 and name CA)	(segid 3A4 and resid 326 and name C)	1.53	0.01	0.02
	assign	(segid 3A4 and resid 326 and name CA)	(segid 3A4 and resid 326 and name CB)	2.40	0.01	0.00
	assign	(segid 3A4 and resid 326 and name CA)	(segid 3A4 and resid 326 and name O)	4.74	0.06	0.06
	assign	(segid 3A4 and resid 326 and name CA)	(segid 3A4 and resid 327 and name C)	3.82	0.01	0.02
	assign	(segid 3A4 and resid 326 and name CA)	(segid 3A4 and resid 327 and name CA)	4.52	0.08	0.07
25	assign	(segid 3A4 and resid 326 and name CA)	(segid 3A4 and resid 327 and name CB)	2.44	0.02	0.01
	assign	(segid 3A4 and resid 326 and name CA)	(segid 3A4 and resid 327 and name N)	4.64	0.07	0.08
	assign	(segid 3A4 and resid 326 and name CA)	(segid 3A4 and resid 327 and name O)	7.40	0.17	0.16
	assign	(segid 3A4 and resid 326 and name CA)	(segid 3A4 and resid 328 and name C)	7.08	0.13	0.13
	assign	(segid 3A4 and resid 326 and name CA)	(segid 3A4 and resid 328 and name CA)	8.36	0.11	0.11
30	assign	(segid 3A4 and resid 326 and name CA)	(segid 3A4 and resid 328 and name CB)	5.96	0.08	0.08
	assign	(segid 3A4 and resid 326 and name CA)	(segid 3A4 and resid 328 and name N)	7.38	0.30	0.29
	assign	(segid 3A4 and resid 326 and name CA)	(segid 3A4 and resid 328 and name O)	8.61	0.10	0.10
	assign	(segid 3A4 and resid 326 and name CA)	(segid 3A4 and resid 329 and name CA)	7.82	0.17	0.18
	assign	(segid 3A4 and resid 326 and name CA)	(segid 3A4 and resid 329 and name CB)	12.15	0.16	0.17
35	assign	(segid 3A4 and resid 326 and name CA)	(segid 3A4 and resid 330 and name CA)	13.24	0.11	0.12
	assign	(segid 3A4 and resid 326 and name CA)	(segid 3A4 and resid 330 and name CB)	13.38	0.42	0.42
	assign	(segid 3A4 and resid 326 and name CA)	(segid 3A4 and resid 331 and name CA)	12.76	0.41	0.41
	assign	(segid 3A4 and resid 326 and name CA)	(segid 3A4 and resid 331 and name CB)	17.08	0.48	0.49
	assign	(segid 3A4 and resid 326 and name CA)	(segid 3A4 and resid 332 and name CA)	17.86	0.55	0.54
40	assign	(segid 3A4 and resid 326 and name CA)	(segid 3A4 and resid 333 and name CA)	15.65	0.27	0.27
	assign	(segid 3A4 and resid 326 and name CA)	(segid 3A4 and resid 335 and name CA)	12.89	0.17	0.17
	assign	(segid 3A4 and resid 326 and name CA)	(segid 3A4 and resid 336 and name CA)	13.54	0.23	0.23
	assign	(segid 3A4 and resid 326 and name CA)	(segid 3A4 and resid 336 and name CB)	9.92	0.21	0.21
	assign	(segid 3A4 and resid 326 and name CA)	(segid 3A4 and resid 337 and name CA)	9.33	0.23	0.22
45	assign	(segid 3A4 and resid 326 and name CA)	(segid 3A4 and resid 337 and name CB)	7.19	0.20	0.21
	assign	(segid 3A4 and resid 326 and name CA)	(segid 3A4 and resid 338 and name C)	8.54	0.25	0.26
	assign	(segid 3A4 and resid 326 and name CA)	(segid 3A4 and resid 338 and name CA)	9.59	0.21	0.20
	assign	(segid 3A4 and resid 326 and name CA)	(segid 3A4 and resid 338 and name CB)	6.94	0.14	0.14
	assign	(segid 3A4 and resid 326 and name CA)	(segid 3A4 and resid 338 and name N)	5.85	0.10	0.10
50	assign	(segid 3A4 and resid 326 and name CA)	(segid 3A4 and resid 339 and name C)	5.38	0.22	0.21
	assign	(segid 3A4 and resid 326 and name CA)	(segid 3A4 and resid 339 and name CA)	5.47	0.24	0.23
	assign	(segid 3A4 and resid 326 and name CA)	(segid 3A4 and resid 339 and name CB)	6.55	0.26	0.26
	assign	(segid 3A4 and resid 326 and name CA)	(segid 3A4 and resid 339 and name N)	7.04	0.10	0.11
	assign	(segid 3A4 and resid 326 and name CA)	(segid 3A4 and resid 339 and name O)	7.03	0.18	0.18
55	assign	(segid 3A4 and resid 326 and name CA)	(segid 3A4 and resid 340 and name C)	6.04	0.20	0.21
	assign	(segid 3A4 and resid 326 and name CA)	(segid 3A4 and resid 340 and name CA)	5.19	0.09	0.09
	assign	(segid 3A4 and resid 326 and name CA)	(segid 3A4 and resid 340 and name N)	8.28	0.18	0.18
	assign	(segid 3A4 and resid 326 and name CA)	(segid 3A4 and resid 341 and name CA)	8.74	0.17	0.17
	assign	(segid 3A4 and resid 326 and name CA)	(segid 3A4 and resid 341 and name CB)	7.11	0.19	0.19
60	assign	(segid 3A4 and resid 326 and name CA)	(segid 3A4 and resid 341 and name N)	7.25	0.18	0.19
	assign	(segid 3A4 and resid 326 and name CA)	(segid 3A4 and resid 342 and name C)	9.83	0.19	0.18
	assign	(segid 3A4 and resid 326 and name CA)	(segid 3A4 and resid 343 and name CA)	11.22	0.25	0.25
	assign	(segid 3A4 and resid 326 and name CA)	(segid 3A4 and resid 343 and name CB)	10.51	0.30	0.31
	assign	(segid 3A4 and resid 326 and name CA)	(segid 3A4 and resid 344 and name CA)	14.49	0.19	0.20
65	assign	(segid 3A4 and resid 326 and name CA)	(segid 3A4 and resid 344 and name CB)	15.61	0.23	0.23
	assign	(segid 3A4 and resid 326 and name CA)	(segid 3A4 and resid 345 and name CA)	15.92	0.25	0.25
	assign	(segid 3A4 and resid 326 and name CA)	(segid 3A4 and resid 345 and name CB)	15.35	0.40	0.40
	assign	(segid 3A4 and resid 326 and name CA)	(segid 3A4 and resid 386 and name CA)	18.20	1.09	1.10
	assign	(segid 3A4 and resid 326 and name CA)	(segid 3A4 and resid 387 and name CA)	16.30	1.15	1.15
70	assign	(segid 3A4 and resid 326 and name CA)	(segid 3A4 and resid 388 and name CA)	15.86	1.23	1.24
	assign	(segid 3A4 and resid 326 and name CA)	(segid 3A4 and resid 388 and name CB)	14.87	1.26	1.26
	assign	(segid 3A4 and resid 326 and name CA)	(segid 3A4 and resid 389 and name CA)	16.15	1.31	1.31
	assign	(segid 3A4 and resid 326 and name CA)	(segid 3A4 and resid 389 and name CB)	15.09	1.33	1.33
	assign	(segid 3A4 and resid 326 and name CB)	(segid 3A4 and resid 327 and name C)	5.70	0.11	0.11
75	assign	(segid 3A4 and resid 326 and name CB)	(segid 3A4 and resid 327 and name CA)	4.65	0.12	0.12
	assign	(segid 3A4 and resid 326 and name CB)	(segid 3A4 and resid 327 and name CB)	4.89	0.09	0.09
	assign	(segid 3A4 and resid 326 and name CB)	(segid 3A4 and resid 327 and name N)	3.38	0.15	0.14
	assign	(segid 3A4 and resid 326 and name CB)	(segid 3A4 and resid 327 and name O)	5.66	0.15	0.15
80	assign	(segid 3A4 and resid 326 and name CB)	(segid 3A4 and resid 328 and name CA)	8.07	0.10	0.10
	assign	(segid 3A4 and resid 326 and name CB)	(segid 3A4 and resid 328 and name CB)	9.35	0.09	0.09
	assign	(segid 3A4 and resid 326 and name CB)	(segid 3A4 and resid 328 and name N)	6.90	0.09	0.09
	assign	(segid 3A4 and resid 326 and name CB)	(segid 3A4 and resid 329 and name CA)	9.28	0.14	0.13

	assign (segid 3A4 and resid 326 and name CB)	(segid 3A4 and resid 329 and name CB)	8.38	0.26	0.26
	assign (segid 3A4 and resid 326 and name CB)	(segid 3A4 and resid 330 and name CA)	12.80	0.24	0.25
	assign (segid 3A4 and resid 326 and name CB)	(segid 3A4 and resid 330 and name CB)	13.86	0.16	0.17
	assign (segid 3A4 and resid 326 and name CB)	(segid 3A4 and resid 331 and name CA)	13.92	0.47	0.47
	assign (segid 3A4 and resid 326 and name CB)	(segid 3A4 and resid 331 and name CB)	13.33	0.45	0.45
5	assign (segid 3A4 and resid 326 and name CB)	(segid 3A4 and resid 332 and name CA)	17.59	0.60	0.61
	assign (segid 3A4 and resid 326 and name CB)	(segid 3A4 and resid 332 and name CB)	18.55	0.72	0.71
	assign (segid 3A4 and resid 326 and name CB)	(segid 3A4 and resid 333 and name CA)	16.60	0.34	0.34
	assign (segid 3A4 and resid 326 and name CB)	(segid 3A4 and resid 333 and name CB)	13.94	0.14	0.14
	assign (segid 3A4 and resid 326 and name CB)	(segid 3A4 and resid 336 and name CA)	14.63	0.20	0.20
10	assign (segid 3A4 and resid 326 and name CB)	(segid 3A4 and resid 336 and name CB)	11.11	0.23	0.24
	assign (segid 3A4 and resid 326 and name CB)	(segid 3A4 and resid 337 and name CA)	10.42	0.26	0.27
	assign (segid 3A4 and resid 326 and name CB)	(segid 3A4 and resid 337 and name CB)	9.95	0.27	0.27
	assign (segid 3A4 and resid 326 and name CB)	(segid 3A4 and resid 338 and name CA)	11.05	0.23	0.22
	assign (segid 3A4 and resid 326 and name CB)	(segid 3A4 and resid 339 and name C)	7.36	0.10	0.10
15	assign (segid 3A4 and resid 326 and name CB)	(segid 3A4 and resid 339 and name CB)	6.86	0.21	0.20
	assign (segid 3A4 and resid 326 and name CB)	(segid 3A4 and resid 340 and name CA)	6.83	0.23	0.23
	assign (segid 3A4 and resid 326 and name CB)	(segid 3A4 and resid 340 and name N)	7.46	0.21	0.21
	assign (segid 3A4 and resid 326 and name CB)	(segid 3A4 and resid 340 and name N)	6.68	0.10	0.11
20	assign (segid 3A4 and resid 326 and name CB)	(segid 3A4 and resid 341 and name CA)	9.65	0.19	0.19
	assign (segid 3A4 and resid 326 and name CB)	(segid 3A4 and resid 341 and name CB)	10.12	0.19	0.18
	assign (segid 3A4 and resid 326 and name CB)	(segid 3A4 and resid 342 and name CA)	10.87	0.19	0.19
	assign (segid 3A4 and resid 326 and name CB)	(segid 3A4 and resid 343 and name CA)	12.01	0.25	0.26
	assign (segid 3A4 and resid 326 and name CB)	(segid 3A4 and resid 343 and name CB)	11.22	0.30	0.31
	assign (segid 3A4 and resid 326 and name CB)	(segid 3A4 and resid 344 and name CA)	15.09	0.19	0.19
25	assign (segid 3A4 and resid 326 and name CB)	(segid 3A4 and resid 344 and name CB)	16.27	0.23	0.24
	assign (segid 3A4 and resid 326 and name CB)	(segid 3A4 and resid 345 and name CA)	16.25	0.25	0.25
	assign (segid 3A4 and resid 326 and name CB)	(segid 3A4 and resid 345 and name CB)	15.55	0.41	0.42
	assign (segid 3A4 and resid 326 and name CB)	(segid 3A4 and resid 346 and name CA)	17.64	1.12	1.11
30	assign (segid 3A4 and resid 326 and name CB)	(segid 3A4 and resid 386 and name CA)	15.50	1.15	1.15
	assign (segid 3A4 and resid 326 and name CB)	(segid 3A4 and resid 387 and name CA)	14.86	1.25	1.26
	assign (segid 3A4 and resid 326 and name CB)	(segid 3A4 and resid 388 and name CA)	13.80	1.28	1.28
	assign (segid 3A4 and resid 326 and name CB)	(segid 3A4 and resid 388 and name CB)	15.36	1.33	1.32
	assign (segid 3A4 and resid 326 and name CB)	(segid 3A4 and resid 389 and name CA)	14.38	1.31	1.32
	assign (segid 3A4 and resid 326 and name CB)	(segid 3A4 and resid 389 and name CB)	18.59	1.28	1.27
35	assign (segid 3A4 and resid 326 and name CB)	(segid 3A4 and resid 390 and name CA)	2.49	0.04	0.05
	assign (segid 3A4 and resid 326 and name N)	(segid 3A4 and resid 326 and name C)	1.47	0.01	0.01
	assign (segid 3A4 and resid 326 and name N)	(segid 3A4 and resid 326 and name CB)	2.47	0.03	0.03
	assign (segid 3A4 and resid 326 and name N)	(segid 3A4 and resid 326 and name O)	3.58	0.04	0.04
40	assign (segid 3A4 and resid 326 and name N)	(segid 3A4 and resid 327 and name C)	4.68	0.08	0.07
	assign (segid 3A4 and resid 326 and name N)	(segid 3A4 and resid 327 and name CA)	4.20	0.10	0.10
	assign (segid 3A4 and resid 326 and name N)	(segid 3A4 and resid 327 and name CB)	5.03	0.06	0.05
	assign (segid 3A4 and resid 326 and name N)	(segid 3A4 and resid 327 and name N)	2.78	0.10	0.11
	assign (segid 3A4 and resid 326 and name N)	(segid 3A4 and resid 327 and name O)	4.22	0.11	0.12
45	assign (segid 3A4 and resid 326 and name N)	(segid 3A4 and resid 328 and name C)	7.01	0.16	0.16
	assign (segid 3A4 and resid 326 and name N)	(segid 3A4 and resid 328 and name CA)	6.83	0.11	0.11
	assign (segid 3A4 and resid 326 and name N)	(segid 3A4 and resid 328 and name N)	5.94	0.08	0.08
	assign (segid 3A4 and resid 326 and name N)	(segid 3A4 and resid 328 and name O)	7.12	0.29	0.29
	assign (segid 3A4 and resid 326 and name N)	(segid 3A4 and resid 329 and name CB)	6.99	0.18	0.19
50	assign (segid 3A4 and resid 326 and name N)	(segid 3A4 and resid 329 and name N)	7.38	0.12	0.12
	assign (segid 3A4 and resid 326 and name N)	(segid 3A4 and resid 329 and name O)	6.65	0.23	0.23
	assign (segid 3A4 and resid 326 and name N)	(segid 3A4 and resid 338 and name C)	6.22	0.20	0.20
	assign (segid 3A4 and resid 326 and name N)	(segid 3A4 and resid 338 and name CB)	5.65	0.13	0.13
	assign (segid 3A4 and resid 326 and name N)	(segid 3A4 and resid 339 and name CA)	5.24	0.22	0.23
	assign (segid 3A4 and resid 326 and name N)	(segid 3A4 and resid 339 and name CB)	5.73	0.21	0.22
55	assign (segid 3A4 and resid 326 and name N)	(segid 3A4 and resid 339 and name N)	6.27	0.27	0.26
	assign (segid 3A4 and resid 326 and name N)	(segid 3A4 and resid 339 and name O)	6.87	0.12	0.11
	assign (segid 3A4 and resid 326 and name N)	(segid 3A4 and resid 340 and name C)	6.46	0.14	0.13
	assign (segid 3A4 and resid 326 and name N)	(segid 3A4 and resid 340 and name CA)	5.75	0.16	0.15
60	assign (segid 3A4 and resid 326 and name N)	(segid 3A4 and resid 340 and name N)	4.91	0.08	0.07
	assign (segid 3A4 and resid 326 and name N)	(segid 3A4 and resid 340 and name O)	7.39	0.12	0.12
	assign (segid 3A4 and resid 326 and name N)	(segid 3A4 and resid 341 and name C)	7.14	0.17	0.17
	assign (segid 3A4 and resid 326 and name N)	(segid 3A4 and resid 341 and name CA)	7.35	0.16	0.16
	assign (segid 3A4 and resid 326 and name N)	(segid 3A4 and resid 341 and name N)	6.34	0.16	0.17
65	assign (segid 3A4 and resid 326 and name N)	(segid 3A4 and resid 341 and name O)	6.11	0.18	0.19
	assign (segid 3A4 and resid 326 and name O)	(segid 3A4 and resid 326 and name CB)	3.02	0.16	0.16
	assign (segid 3A4 and resid 326 and name O)	(segid 3A4 and resid 327 and name C)	4.16	0.08	0.07
	assign (segid 3A4 and resid 326 and name O)	(segid 3A4 and resid 327 and name CA)	2.81	0.02	0.03
	assign (segid 3A4 and resid 326 and name O)	(segid 3A4 and resid 327 and name CB)	3.30	0.31	0.30
	assign (segid 3A4 and resid 326 and name O)	(segid 3A4 and resid 327 and name N)	2.24	0.01	0.02
70	assign (segid 3A4 and resid 326 and name O)	(segid 3A4 and resid 327 and name O)	4.68	0.09	0.10
	assign (segid 3A4 and resid 326 and name O)	(segid 3A4 and resid 328 and name C)	6.96	0.22	0.21
	assign (segid 3A4 and resid 326 and name O)	(segid 3A4 and resid 328 and name CA)	6.40	0.13	0.14
	assign (segid 3A4 and resid 326 and name O)	(segid 3A4 and resid 328 and name CB)	7.39	0.12	0.12
	assign (segid 3A4 and resid 326 and name O)	(segid 3A4 and resid 328 and name N)	5.04	0.11	0.10
75	assign (segid 3A4 and resid 326 and name O)	(segid 3A4 and resid 328 and name O)	6.81	0.38	0.38
	assign (segid 3A4 and resid 326 and name O)	(segid 3A4 and resid 338 and name C)	7.17	0.28	0.28
	assign (segid 3A4 and resid 326 and name O)	(segid 3A4 and resid 338 and name CB)	5.82	0.41	0.40
	assign (segid 3A4 and resid 326 and name O)	(segid 3A4 and resid 339 and name CA)	5.04	0.34	0.35
	assign (segid 3A4 and resid 326 and name O)	(segid 3A4 and resid 339 and name CB)	4.50	0.36	0.35
80	assign (segid 3A4 and resid 326 and name O)	(segid 3A4 and resid 339 and name N)	6.18	0.29	0.30
	assign (segid 3A4 and resid 326 and name O)	(segid 3A4 and resid 339 and name O)	6.90	0.40	0.39
	assign (segid 3A4 and resid 326 and name O)	(segid 3A4 and resid 340 and name CA)	6.66	0.56	0.55

	assign (segid 3A4 and resid 326 and name O) (segid 3A4 and resid 340 and name N)	5.59	0.48	0.49
	assign (segid 3A4 and resid 327 and name C) (segid 3A4 and resid 327 and name CB)	2.49	0.02	0.02
	assign (segid 3A4 and resid 327 and name C) (segid 3A4 and resid 327 and name O)	1.23	0.01	0.01
	assign (segid 3A4 and resid 327 and name C) (segid 3A4 and resid 328 and name C)	3.00	0.09	0.09
5	assign (segid 3A4 and resid 327 and name C) (segid 3A4 and resid 328 and name CA)	2.44	0.02	0.02
	assign (segid 3A4 and resid 327 and name C) (segid 3A4 and resid 328 and name CB)	3.70	0.05	0.05
	assign (segid 3A4 and resid 327 and name C) (segid 3A4 and resid 328 and name N)	1.33	0.00	0.01
	assign (segid 3A4 and resid 327 and name C) (segid 3A4 and resid 328 and name O)	3.22	0.10	0.10
	assign (segid 3A4 and resid 327 and name C) (segid 3A4 and resid 329 and name C)	6.23	0.17	0.16
10	assign (segid 3A4 and resid 327 and name C) (segid 3A4 and resid 329 and name CA)	4.94	0.19	0.19
	assign (segid 3A4 and resid 327 and name C) (segid 3A4 and resid 329 and name CB)	4.92	0.28	0.29
	assign (segid 3A4 and resid 327 and name C) (segid 3A4 and resid 329 and name N)	3.91	0.14	0.14
	assign (segid 3A4 and resid 327 and name C) (segid 3A4 and resid 329 and name O)	6.46	0.17	0.16
15	assign (segid 3A4 and resid 327 and name C) (segid 3A4 and resid 330 and name N)	7.28	0.17	0.17
	assign (segid 3A4 and resid 327 and name C) (segid 3A4 and resid 337 and name C)	5.74	0.22	0.22
	assign (segid 3A4 and resid 327 and name C) (segid 3A4 and resid 337 and name CA)	6.91	0.21	0.21
	assign (segid 3A4 and resid 327 and name C) (segid 3A4 and resid 337 and name CB)	6.84	0.25	0.24
	assign (segid 3A4 and resid 327 and name C) (segid 3A4 and resid 337 and name N)	7.40	0.16	0.15
20	assign (segid 3A4 and resid 327 and name C) (segid 3A4 and resid 337 and name O)	4.82	0.23	0.22
	assign (segid 3A4 and resid 327 and name C) (segid 3A4 and resid 338 and name C)	4.70	0.21	0.22
	assign (segid 3A4 and resid 327 and name C) (segid 3A4 and resid 338 and name CA)	5.44	0.34	0.34
	assign (segid 3A4 and resid 327 and name C) (segid 3A4 and resid 338 and name CB)	6.68	0.35	0.36
	assign (segid 3A4 and resid 327 and name C) (segid 3A4 and resid 338 and name N)	6.06	0.29	0.29
	assign (segid 3A4 and resid 327 and name C) (segid 3A4 and resid 338 and name O)	5.16	0.09	0.10
25	assign (segid 3A4 and resid 327 and name C) (segid 3A4 and resid 339 and name C)	5.25	0.18	0.18
	assign (segid 3A4 and resid 327 and name C) (segid 3A4 and resid 339 and name CA)	3.83	0.19	0.19
	assign (segid 3A4 and resid 327 and name C) (segid 3A4 and resid 339 and name CB)	3.90	0.25	0.26
	assign (segid 3A4 and resid 327 and name C) (segid 3A4 and resid 339 and name N)	3.99	0.29	0.30
	assign (segid 3A4 and resid 327 and name C) (segid 3A4 and resid 339 and name O)	6.19	0.19	0.20
30	assign (segid 3A4 and resid 327 and name C) (segid 3A4 and resid 340 and name CA)	7.06	0.23	0.23
	assign (segid 3A4 and resid 327 and name C) (segid 3A4 and resid 340 and name N)	5.63	0.21	0.21
	assign (segid 3A4 and resid 327 and name C) (segid 3A4 and resid 341 and name N)	7.33	0.16	0.15
	assign (segid 3A4 and resid 327 and name CA) (segid 3A4 and resid 327 and name C)	1.52	0.00	0.01
	assign (segid 3A4 and resid 327 and name CA) (segid 3A4 and resid 327 and name CB)	1.53	0.01	0.00
35	assign (segid 3A4 and resid 327 and name CA) (segid 3A4 and resid 327 and name O)	2.39	0.02	0.02
	assign (segid 3A4 and resid 327 and name CA) (segid 3A4 and resid 328 and name C)	4.34	0.08	0.07
	assign (segid 3A4 and resid 327 and name CA) (segid 3A4 and resid 328 and name CA)	3.81	0.03	0.03
	assign (segid 3A4 and resid 327 and name CA) (segid 3A4 and resid 328 and name CB)	4.86	0.04	0.04
	assign (segid 3A4 and resid 327 and name CA) (segid 3A4 and resid 328 and name N)	2.44	0.03	0.03
40	assign (segid 3A4 and resid 327 and name CA) (segid 3A4 and resid 328 and name O)	4.26	0.12	0.12
	assign (segid 3A4 and resid 327 and name CA) (segid 3A4 and resid 329 and name C)	7.61	0.15	0.14
	assign (segid 3A4 and resid 327 and name CA) (segid 3A4 and resid 329 and name CA)	6.24	0.16	0.16
	assign (segid 3A4 and resid 327 and name CA) (segid 3A4 and resid 329 and name CB)	6.07	0.28	0.28
	assign (segid 3A4 and resid 327 and name CA) (segid 3A4 and resid 329 and name N)	5.33	0.11	0.12
45	assign (segid 3A4 and resid 327 and name CA) (segid 3A4 and resid 330 and name CA)	9.94	0.15	0.14
	assign (segid 3A4 and resid 327 and name CA) (segid 3A4 and resid 330 and name CB)	10.74	0.13	0.13
	assign (segid 3A4 and resid 327 and name CA) (segid 3A4 and resid 331 and name CA)	12.12	0.22	0.21
	assign (segid 3A4 and resid 327 and name CA) (segid 3A4 and resid 331 and name CB)	11.86	0.32	0.32
	assign (segid 3A4 and resid 327 and name CA) (segid 3A4 and resid 332 and name CA)	15.72	0.22	0.22
50	assign (segid 3A4 and resid 327 and name CA) (segid 3A4 and resid 333 and name CA)	15.82	0.54	0.54
	assign (segid 3A4 and resid 327 and name CA) (segid 3A4 and resid 335 and name CA)	13.80	0.30	0.30
	assign (segid 3A4 and resid 327 and name CA) (segid 3A4 and resid 336 and name CA)	10.58	0.25	0.26
	assign (segid 3A4 and resid 327 and name CA) (segid 3A4 and resid 336 and name CB)	10.94	0.37	0.37
	assign (segid 3A4 and resid 327 and name CA) (segid 3A4 and resid 337 and name C)	7.16	0.23	0.22
55	assign (segid 3A4 and resid 327 and name CA) (segid 3A4 and resid 337 and name CA)	8.34	0.22	0.22
	assign (segid 3A4 and resid 327 and name CA) (segid 3A4 and resid 337 and name CB)	8.19	0.25	0.24
	assign (segid 3A4 and resid 327 and name CA) (segid 3A4 and resid 337 and name O)	6.29	0.23	0.23
	assign (segid 3A4 and resid 327 and name CA) (segid 3A4 and resid 338 and name C)	5.69	0.26	0.25
	assign (segid 3A4 and resid 327 and name CA) (segid 3A4 and resid 338 and name CA)	6.62	0.35	0.35
60	assign (segid 3A4 and resid 327 and name CA) (segid 3A4 and resid 338 and name CB)	7.75	0.39	0.38
	assign (segid 3A4 and resid 327 and name CA) (segid 3A4 and resid 339 and name C)	6.07	0.12	0.12
	assign (segid 3A4 and resid 327 and name CA) (segid 3A4 and resid 339 and name CA)	5.48	0.18	0.19
	assign (segid 3A4 and resid 327 and name CA) (segid 3A4 and resid 339 and name CB)	4.18	0.22	0.23
	assign (segid 3A4 and resid 327 and name CA) (segid 3A4 and resid 339 and name N)	3.86	0.29	0.29
65	assign (segid 3A4 and resid 327 and name CA) (segid 3A4 and resid 339 and name O)	4.77	0.33	0.34
	assign (segid 3A4 and resid 327 and name CA) (segid 3A4 and resid 340 and name CA)	6.50	0.23	0.24
	assign (segid 3A4 and resid 327 and name CA) (segid 3A4 and resid 340 and name N)	7.07	0.20	0.20
	assign (segid 3A4 and resid 327 and name CA) (segid 3A4 and resid 341 and name CA)	5.70	0.17	0.17
	assign (segid 3A4 and resid 327 and name CA) (segid 3A4 and resid 341 and name CB)	8.96	0.11	0.11
70	assign (segid 3A4 and resid 327 and name CA) (segid 3A4 and resid 341 and name N)	8.91	0.11	0.11
	assign (segid 3A4 and resid 327 and name CA) (segid 3A4 and resid 342 and name CA)	11.51	0.23	0.22
	assign (segid 3A4 and resid 327 and name CA) (segid 3A4 and resid 343 and name CA)	12.73	0.35	0.35
	assign (segid 3A4 and resid 327 and name CA) (segid 3A4 and resid 343 and name CB)	11.90	0.43	0.43
	assign (segid 3A4 and resid 327 and name CA) (segid 3A4 and resid 344 and name CA)	16.31	0.34	0.35
75	assign (segid 3A4 and resid 327 and name CA) (segid 3A4 and resid 344 and name CB)	17.38	0.31	0.31
	assign (segid 3A4 and resid 327 and name CA) (segid 3A4 and resid 345 and name CA)	17.65	0.56	0.57
	assign (segid 3A4 and resid 327 and name CA) (segid 3A4 and resid 345 and name CB)	17.18	0.68	0.68
	assign (segid 3A4 and resid 327 and name CA) (segid 3A4 and resid 387 and name CA)	18.52	0.73	0.73
	assign (segid 3A4 and resid 327 and name CA) (segid 3A4 and resid 388 and name CA)	18.50	0.98	0.98
80	assign (segid 3A4 and resid 327 and name CA) (segid 3A4 and resid 388 and name CB)	17.52	1.08	1.08
	assign (segid 3A4 and resid 327 and name CA) (segid 3A4 and resid 389 and name CB)	18.18	1.06	1.07
	assign (segid 3A4 and resid 327 and name CB) (segid 3A4 and resid 328 and name C)	4.53	0.11	0.11
	assign (segid 3A4 and resid 327 and name CB) (segid 3A4 and resid 328 and name CA)	4.35	0.10	0.10

	assign (segid 3A4 and resid 327 and name CB)	(segid 3A4 and resid 328 and name CB)	5.25	0.10	0.11
	assign (segid 3A4 and resid 327 and name CB)	(segid 3A4 and resid 328 and name N)	3.02	0.13	0.13
	assign (segid 3A4 and resid 327 and name CB)	(segid 3A4 and resid 328 and name O)	4.04	0.19	0.18
	assign (segid 3A4 and resid 327 and name CB)	(segid 3A4 and resid 329 and name CA)	6.32	0.19	0.20
5	assign (segid 3A4 and resid 327 and name CB)	(segid 3A4 and resid 329 and name CB)	6.16	0.32	0.32
	assign (segid 3A4 and resid 327 and name CB)	(segid 3A4 and resid 329 and name N)	5.64	0.12	0.12
	assign (segid 3A4 and resid 327 and name CB)	(segid 3A4 and resid 330 and name CA)	10.01	0.20	0.19
	assign (segid 3A4 and resid 327 and name CB)	(segid 3A4 and resid 330 and name CB)	10.69	0.21	0.21
	assign (segid 3A4 and resid 327 and name CB)	(segid 3A4 and resid 331 and name CA)	12.30	0.28	0.28
10	assign (segid 3A4 and resid 327 and name CB)	(segid 3A4 and resid 331 and name CB)	12.17	0.40	0.41
	assign (segid 3A4 and resid 327 and name CB)	(segid 3A4 and resid 332 and name CA)	15.85	0.25	0.25
	assign (segid 3A4 and resid 327 and name CB)	(segid 3A4 and resid 333 and name CA)	15.97	0.63	0.64
	assign (segid 3A4 and resid 327 and name CB)	(segid 3A4 and resid 335 and name CA)	14.32	0.35	0.34
	assign (segid 3A4 and resid 327 and name CB)	(segid 3A4 and resid 336 and name CA)	11.16	0.28	0.28
	assign (segid 3A4 and resid 327 and name CB)	(segid 3A4 and resid 336 and name CB)	11.48	0.41	0.41
15	assign (segid 3A4 and resid 327 and name CB)	(segid 3A4 and resid 337 and name CA)	9.28	0.22	0.21
	assign (segid 3A4 and resid 327 and name CB)	(segid 3A4 and resid 337 and name CB)	9.10	0.29	0.28
	assign (segid 3A4 and resid 327 and name CB)	(segid 3A4 and resid 337 and name O)	7.19	0.23	0.23
	assign (segid 3A4 and resid 327 and name CB)	(segid 3A4 and resid 338 and name C)	7.05	0.22	0.23
	assign (segid 3A4 and resid 327 and name CB)	(segid 3A4 and resid 338 and name CA)	7.85	0.33	0.33
20	assign (segid 3A4 and resid 327 and name CB)	(segid 3A4 and resid 338 and name CB)	9.01	0.39	0.38
	assign (segid 3A4 and resid 327 and name CB)	(segid 3A4 and resid 338 and name O)	7.48	0.11	0.10
	assign (segid 3A4 and resid 327 and name CB)	(segid 3A4 and resid 339 and name C)	6.99	0.18	0.18
	assign (segid 3A4 and resid 327 and name CB)	(segid 3A4 and resid 339 and name CA)	5.67	0.21	0.21
	assign (segid 3A4 and resid 327 and name CB)	(segid 3A4 and resid 339 and name CB)	5.22	0.28	0.29
25	assign (segid 3A4 and resid 327 and name CB)	(segid 3A4 and resid 339 and name N)	6.16	0.31	0.31
	assign (segid 3A4 and resid 327 and name CB)	(segid 3A4 and resid 340 and name CA)	8.54	0.19	0.19
	assign (segid 3A4 and resid 327 and name CB)	(segid 3A4 and resid 340 and name N)	7.19	0.16	0.16
	assign (segid 3A4 and resid 327 and name CB)	(segid 3A4 and resid 341 and name CA)	10.40	0.12	0.12
30	assign (segid 3A4 and resid 327 and name CB)	(segid 3A4 and resid 341 and name CB)	10.30	0.15	0.15
	assign (segid 3A4 and resid 327 and name CB)	(segid 3A4 and resid 342 and name CA)	12.81	0.22	0.22
	assign (segid 3A4 and resid 327 and name CB)	(segid 3A4 and resid 343 and name CA)	13.79	0.40	0.41
	assign (segid 3A4 and resid 327 and name CB)	(segid 3A4 and resid 343 and name CB)	12.86	0.49	0.49
	assign (segid 3A4 and resid 327 and name CB)	(segid 3A4 and resid 344 and name CA)	17.29	0.40	0.40
35	assign (segid 3A4 and resid 327 and name CB)	(segid 3A4 and resid 344 and name CB)	18.43	0.36	0.35
	assign (segid 3A4 and resid 327 and name CB)	(segid 3A4 and resid 345 and name CA)	18.38	0.64	0.63
	assign (segid 3A4 and resid 327 and name CB)	(segid 3A4 and resid 345 and name CB)	17.81	0.72	0.73
	assign (segid 3A4 and resid 327 and name CB)	(segid 3A4 and resid 387 and name CA)	18.35	0.74	0.75
	assign (segid 3A4 and resid 327 and name CB)	(segid 3A4 and resid 388 and name CA)	18.28	1.05	1.05
40	assign (segid 3A4 and resid 327 and name CB)	(segid 3A4 and resid 388 and name CB)	17.25	1.15	1.15
	assign (segid 3A4 and resid 327 and name CB)	(segid 3A4 and resid 389 and name CB)	18.35	1.05	1.05
	assign (segid 3A4 and resid 327 and name N)	(segid 3A4 and resid 327 and name C)	2.39	0.04	0.03
	assign (segid 3A4 and resid 327 and name N)	(segid 3A4 and resid 327 and name CB)	1.45	0.00	0.01
	assign (segid 3A4 and resid 327 and name N)	(segid 3A4 and resid 327 and name O)	2.44	0.02	0.02
45	assign (segid 3A4 and resid 327 and name N)	(segid 3A4 and resid 328 and name C)	2.60	0.04	0.05
	assign (segid 3A4 and resid 327 and name N)	(segid 3A4 and resid 328 and name CA)	5.19	0.05	0.05
	assign (segid 3A4 and resid 327 and name N)	(segid 3A4 and resid 328 and name CB)	4.81	0.07	0.06
	assign (segid 3A4 and resid 327 and name N)	(segid 3A4 and resid 328 and name N)	6.04	0.08	0.07
	assign (segid 3A4 and resid 327 and name N)	(segid 3A4 and resid 328 and name O)	3.60	0.04	0.04
50	assign (segid 3A4 and resid 327 and name N)	(segid 3A4 and resid 329 and name O)	5.17	0.13	0.13
	assign (segid 3A4 and resid 327 and name N)	(segid 3A4 and resid 329 and name CA)	6.74	0.10	0.10
	assign (segid 3A4 and resid 327 and name N)	(segid 3A4 and resid 329 and name CB)	6.25	0.23	0.24
	assign (segid 3A4 and resid 327 and name N)	(segid 3A4 and resid 329 and name N)	5.97	0.07	0.07
	assign (segid 3A4 and resid 327 and name N)	(segid 3A4 and resid 337 and name O)	6.72	0.29	0.28
	assign (segid 3A4 and resid 327 and name N)	(segid 3A4 and resid 338 and name C)	5.87	0.29	0.29
55	assign (segid 3A4 and resid 327 and name N)	(segid 3A4 and resid 338 and name CA)	7.01	0.36	0.36
	assign (segid 3A4 and resid 327 and name N)	(segid 3A4 and resid 338 and name O)	5.96	0.17	0.17
	assign (segid 3A4 and resid 327 and name N)	(segid 3A4 and resid 339 and name C)	5.27	0.23	0.23
	assign (segid 3A4 and resid 327 and name N)	(segid 3A4 and resid 339 and name CA)	4.23	0.30	0.30
60	assign (segid 3A4 and resid 327 and name N)	(segid 3A4 and resid 339 and name CB)	4.18	0.35	0.36
	assign (segid 3A4 and resid 327 and name N)	(segid 3A4 and resid 339 and name N)	5.09	0.37	0.38
	assign (segid 3A4 and resid 327 and name N)	(segid 3A4 and resid 339 and name O)	6.42	0.26	0.26
	assign (segid 3A4 and resid 327 and name N)	(segid 3A4 and resid 340 and name C)	7.38	0.17	0.16
	assign (segid 3A4 and resid 327 and name N)	(segid 3A4 and resid 340 and name CA)	6.41	0.21	0.20
65	assign (segid 3A4 and resid 327 and name N)	(segid 3A4 and resid 340 and name N)	5.15	0.18	0.17
	assign (segid 3A4 and resid 327 and name N)	(segid 3A4 and resid 341 and name N)	7.18	0.15	0.15
	assign (segid 3A4 and resid 327 and name O)	(segid 3A4 and resid 327 and name CB)	3.37	0.09	0.09
	assign (segid 3A4 and resid 327 and name O)	(segid 3A4 and resid 328 and name C)	3.04	0.16	0.17
	assign (segid 3A4 and resid 327 and name O)	(segid 3A4 and resid 328 and name CA)	2.77	0.04	0.04
70	assign (segid 3A4 and resid 327 and name O)	(segid 3A4 and resid 328 and name CB)	4.22	0.09	0.10
	assign (segid 3A4 and resid 327 and name O)	(segid 3A4 and resid 328 and name N)	2.25	0.02	0.03
	assign (segid 3A4 and resid 327 and name O)	(segid 3A4 and resid 329 and name C)	3.47	0.18	0.18
	assign (segid 3A4 and resid 327 and name O)	(segid 3A4 and resid 329 and name CA)	5.70	0.31	0.30
	assign (segid 3A4 and resid 327 and name O)	(segid 3A4 and resid 329 and name CB)	4.49	0.34	0.34
	assign (segid 3A4 and resid 327 and name O)	(segid 3A4 and resid 329 and name N)	4.24	0.44	0.44
75	assign (segid 3A4 and resid 327 and name O)	(segid 3A4 and resid 329 and name O)	3.56	0.25	0.26
	assign (segid 3A4 and resid 327 and name O)	(segid 3A4 and resid 330 and name N)	5.85	0.27	0.27
	assign (segid 3A4 and resid 327 and name O)	(segid 3A4 and resid 330 and name O)	6.80	0.33	0.33
	assign (segid 3A4 and resid 327 and name O)	(segid 3A4 and resid 337 and name C)	5.09	0.26	0.27
80	assign (segid 3A4 and resid 327 and name O)	(segid 3A4 and resid 337 and name CA)	6.13	0.24	0.25
	assign (segid 3A4 and resid 327 and name O)	(segid 3A4 and resid 337 and name CB)	5.87	0.27	0.28
	assign (segid 3A4 and resid 327 and name O)	(segid 3A4 and resid 337 and name N)	6.72	0.17	0.17
	assign (segid 3A4 and resid 327 and name O)	(segid 3A4 and resid 337 and name O)	4.27	0.27	0.26

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	assign (segid 3A4 and resid 327 and name O) (segid 3A4 and resid 338 and name C)	4.32	0.39	0.39
	assign (segid 3A4 and resid 327 and name O) (segid 3A4 and resid 338 and name CA)	5.11	0.44	0.45
	assign (segid 3A4 and resid 327 and name O) (segid 3A4 and resid 338 and name CB)	6.46	0.43	0.44
	assign (segid 3A4 and resid 327 and name O) (segid 3A4 and resid 338 and name N)	5.50	0.36	0.37
5	assign (segid 3A4 and resid 327 and name O) (segid 3A4 and resid 338 and name O)	4.56	0.27	0.28
	assign (segid 3A4 and resid 327 and name O) (segid 3A4 and resid 339 and name C)	5.09	0.41	0.41
	assign (segid 3A4 and resid 327 and name O) (segid 3A4 and resid 339 and name CA)	3.80	0.44	0.45
	assign (segid 3A4 and resid 327 and name O) (segid 3A4 and resid 339 and name CB)	4.32	0.47	0.47
	assign (segid 3A4 and resid 327 and name O) (segid 3A4 and resid 339 and name N)	3.90	0.50	0.51
	assign (segid 3A4 and resid 327 and name O) (segid 3A4 and resid 340 and name C)	6.08	0.42	0.41
10	assign (segid 3A4 and resid 327 and name O) (segid 3A4 and resid 340 and name CA)	7.29	0.34	0.35
	assign (segid 3A4 and resid 327 and name O) (segid 3A4 and resid 340 and name N)	6.71	0.39	0.39
	assign (segid 3A4 and resid 327 and name O) (segid 3A4 and resid 341 and name CB)	5.33	0.40	0.39
	assign (segid 3A4 and resid 327 and name O) (segid 3A4 and resid 341 and name N)	7.25	0.26	0.25
15	assign (segid 3A4 and resid 327 and name O) (segid 3A4 and resid 341 and name O)	6.67	0.30	0.29
	assign (segid 3A4 and resid 327 and name O) (segid 3A4 and resid 342 and name C)	7.35	0.15	0.15
	assign (segid 3A4 and resid 327 and name O) (segid 3A4 and resid 342 and name CB)	2.50	0.03	0.04
	assign (segid 3A4 and resid 328 and name C) (segid 3A4 and resid 328 and name O)	1.24	0.01	0.00
	assign (segid 3A4 and resid 328 and name C) (segid 3A4 and resid 329 and name C)	3.62	0.03	0.03
20	assign (segid 3A4 and resid 328 and name C) (segid 3A4 and resid 329 and name CB)	2.42	0.00	0.01
	assign (segid 3A4 and resid 328 and name C) (segid 3A4 and resid 329 and name N)	3.22	0.11	0.10
	assign (segid 3A4 and resid 328 and name C) (segid 3A4 and resid 329 and name O)	1.33	0.01	0.00
	assign (segid 3A4 and resid 328 and name C) (segid 3A4 and resid 329 and name O)	4.03	0.06	0.06
	assign (segid 3A4 and resid 328 and name C) (segid 3A4 and resid 330 and name C)	6.90	0.08	0.07
25	assign (segid 3A4 and resid 328 and name C) (segid 3A4 and resid 330 and name CA)	5.87	0.09	0.09
	assign (segid 3A4 and resid 328 and name C) (segid 3A4 and resid 330 and name CB)	6.54	0.12	0.12
	assign (segid 3A4 and resid 328 and name C) (segid 3A4 and resid 330 and name N)	4.59	0.11	0.11
	assign (segid 3A4 and resid 328 and name C) (segid 3A4 and resid 330 and name O)	7.34	0.23	0.22
	assign (segid 3A4 and resid 328 and name C) (segid 3A4 and resid 331 and name CB)	7.52	0.25	0.24
30	assign (segid 3A4 and resid 328 and name C) (segid 3A4 and resid 331 and name N)	6.51	0.27	0.27
	assign (segid 3A4 and resid 328 and name C) (segid 3A4 and resid 336 and name C)	6.75	0.30	0.31
	assign (segid 3A4 and resid 328 and name C) (segid 3A4 and resid 336 and name CA)	7.09	0.39	0.38
	assign (segid 3A4 and resid 328 and name C) (segid 3A4 and resid 336 and name CB)	4.79	0.13	0.13
	assign (segid 3A4 and resid 328 and name C) (segid 3A4 and resid 337 and name C)	5.68	0.15	0.14
35	assign (segid 3A4 and resid 328 and name C) (segid 3A4 and resid 337 and name CB)	5.80	0.21	0.20
	assign (segid 3A4 and resid 328 and name C) (segid 3A4 and resid 337 and name N)	5.58	0.13	0.13
	assign (segid 3A4 and resid 328 and name C) (segid 3A4 and resid 337 and name O)	3.61	0.14	0.14
	assign (segid 3A4 and resid 328 and name C) (segid 3A4 and resid 338 and name C)	5.50	0.10	0.10
	assign (segid 3A4 and resid 328 and name C) (segid 3A4 and resid 338 and name CA)	6.47	0.18	0.18
40	assign (segid 3A4 and resid 328 and name C) (segid 3A4 and resid 338 and name CB)	6.81	0.25	0.24
	assign (segid 3A4 and resid 328 and name C) (segid 3A4 and resid 338 and name N)	5.60	0.15	0.15
	assign (segid 3A4 and resid 328 and name C) (segid 3A4 and resid 338 and name O)	6.10	0.23	0.24
	assign (segid 3A4 and resid 328 and name C) (segid 3A4 and resid 339 and name C)	7.27	0.18	0.18
	assign (segid 3A4 and resid 328 and name C) (segid 3A4 and resid 339 and name CA)	5.87	0.19	0.18
45	assign (segid 3A4 and resid 328 and name C) (segid 3A4 and resid 339 and name CB)	6.20	0.21	0.21
	assign (segid 3A4 and resid 328 and name C) (segid 3A4 and resid 339 and name N)	5.30	0.04	0.04
	assign (segid 3A4 and resid 328 and name C) (segid 3A4 and resid 339 and name O)	1.52	0.01	0.00
	assign (segid 3A4 and resid 328 and name CA) (segid 3A4 and resid 328 and name CB)	1.52	0.01	0.02
	assign (segid 3A4 and resid 328 and name CA) (segid 3A4 and resid 328 and name O)	2.39	0.02	0.02
50	assign (segid 3A4 and resid 328 and name CA) (segid 3A4 and resid 329 and name C)	4.79	0.03	0.03
	assign (segid 3A4 and resid 328 and name CA) (segid 3A4 and resid 329 and name CA)	3.79	0.02	0.02
	assign (segid 3A4 and resid 328 and name CA) (segid 3A4 and resid 329 and name CB)	4.51	0.12	0.12
	assign (segid 3A4 and resid 328 and name CA) (segid 3A4 and resid 329 and name N)	2.43	0.04	0.03
	assign (segid 3A4 and resid 328 and name CA) (segid 3A4 and resid 329 and name O)	4.90	0.05	0.04
55	assign (segid 3A4 and resid 328 and name CA) (segid 3A4 and resid 330 and name CA)	7.01	0.11	0.12
	assign (segid 3A4 and resid 328 and name CA) (segid 3A4 and resid 330 and name CB)	7.66	0.15	0.15
	assign (segid 3A4 and resid 328 and name CA) (segid 3A4 and resid 330 and name N)	5.85	0.12	0.13
	assign (segid 3A4 and resid 328 and name CA) (segid 3A4 and resid 331 and name CA)	9.83	0.23	0.22
	assign (segid 3A4 and resid 328 and name CA) (segid 3A4 and resid 331 and name CB)	9.83	0.30	0.31
60	assign (segid 3A4 and resid 328 and name CA) (segid 3A4 and resid 332 and name CA)	13.17	0.20	0.19
	assign (segid 3A4 and resid 328 and name CA) (segid 3A4 and resid 333 and name CA)	12.69	0.34	0.33
	assign (segid 3A4 and resid 328 and name CA) (segid 3A4 and resid 335 and name CA)	10.57	0.28	0.28
	assign (segid 3A4 and resid 328 and name CA) (segid 3A4 and resid 336 and name C)	6.64	0.30	0.29
	assign (segid 3A4 and resid 328 and name CA) (segid 3A4 and resid 336 and name CA)	7.09	0.32	0.32
65	assign (segid 3A4 and resid 328 and name CA) (segid 3A4 and resid 336 and name CB)	7.26	0.42	0.42
	assign (segid 3A4 and resid 328 and name CA) (segid 3A4 and resid 337 and name C)	4.45	0.14	0.14
	assign (segid 3A4 and resid 328 and name CA) (segid 3A4 and resid 337 and name CA)	5.66	0.14	0.14
	assign (segid 3A4 and resid 328 and name CA) (segid 3A4 and resid 337 and name CB)	6.01	0.18	0.18
	assign (segid 3A4 and resid 328 and name CA) (segid 3A4 and resid 337 and name N)	5.79	0.13	0.12
70	assign (segid 3A4 and resid 328 and name CA) (segid 3A4 and resid 337 and name O)	3.35	0.15	0.15
	assign (segid 3A4 and resid 328 and name CA) (segid 3A4 and resid 338 and name C)	4.43	0.11	0.12
	assign (segid 3A4 and resid 328 and name CA) (segid 3A4 and resid 338 and name CA)	4.46	0.21	0.21
	assign (segid 3A4 and resid 328 and name CA) (segid 3A4 and resid 338 and name CB)	5.69	0.29	0.29
	assign (segid 3A4 and resid 328 and name CA) (segid 3A4 and resid 338 and name N)	4.94	0.17	0.16
75	assign (segid 3A4 and resid 328 and name CA) (segid 3A4 and resid 338 and name O)	5.23	0.24	0.23
	assign (segid 3A4 and resid 328 and name CA) (segid 3A4 and resid 339 and name C)	6.11	0.20	0.20
	assign (segid 3A4 and resid 328 and name CA) (segid 3A4 and resid 339 and name CA)	4.67	0.21	0.21
	assign (segid 3A4 and resid 328 and name CA) (segid 3A4 and resid 339 and name CB)	4.89	0.24	0.24
	assign (segid 3A4 and resid 328 and name CA) (segid 3A4 and resid 339 and name N)	4.03	0.06	0.06
80	assign (segid 3A4 and resid 328 and name CA) (segid 3A4 and resid 339 and name O)	6.73	0.16	0.16
	assign (segid 3A4 and resid 328 and name CA) (segid 3A4 and resid 340 and name CA)	8.24	0.25	0.26
	assign (segid 3A4 and resid 328 and name CA) (segid 3A4 and resid 340 and name N)	6.83	0.26	0.26
	assign (segid 3A4 and resid 328 and name CA) (segid 3A4 and resid 341 and name CA)	8.84	0.18	0.18

	assign (segid 3A4 and resid 328 and name CA)	(segid 3A4 and resid 341 and name CB)	8.19	0.18	0.19
	assign (segid 3A4 and resid 328 and name CA)	(segid 3A4 and resid 342 and name CA)	11.80	0.25	0.24
	assign (segid 3A4 and resid 328 and name CA)	(segid 3A4 and resid 343 and name CA)	12.60	0.47	0.48
	assign (segid 3A4 and resid 328 and name CA)	(segid 3A4 and resid 343 and name CB)	11.74	0.56	0.57
5	assign (segid 3A4 and resid 328 and name CA)	(segid 3A4 and resid 344 and name CA)	16.27	0.51	0.51
	assign (segid 3A4 and resid 328 and name CA)	(segid 3A4 and resid 344 and name CB)	17.24	0.48	0.48
	assign (segid 3A4 and resid 328 and name CA)	(segid 3A4 and resid 345 and name CA)	17.57	0.74	0.73
	assign (segid 3A4 and resid 328 and name CA)	(segid 3A4 and resid 345 and name CB)	17.28	0.81	0.82
	assign (segid 3A4 and resid 328 and name CB)	(segid 3A4 and resid 329 and name C)	5.36	0.10	0.11
10	assign (segid 3A4 and resid 328 and name CB)	(segid 3A4 and resid 329 and name CA)	4.61	0.05	0.04
	assign (segid 3A4 and resid 328 and name CB)	(segid 3A4 and resid 329 and name CB)	5.63	0.08	0.09
	assign (segid 3A4 and resid 328 and name CB)	(segid 3A4 and resid 329 and name N)	3.31	0.07	0.07
	assign (segid 3A4 and resid 328 and name CB)	(segid 3A4 and resid 329 and name O)	5.42	0.10	0.10
	assign (segid 3A4 and resid 328 and name CB)	(segid 3A4 and resid 330 and name CA)	7.33	0.25	0.24
15	assign (segid 3A4 and resid 328 and name CB)	(segid 3A4 and resid 330 and name CB)	7.71	0.30	0.29
	assign (segid 3A4 and resid 328 and name CB)	(segid 3A4 and resid 330 and name N)	6.30	0.23	0.23
	assign (segid 3A4 and resid 328 and name CB)	(segid 3A4 and resid 331 and name CA)	10.50	0.30	0.29
	assign (segid 3A4 and resid 328 and name CB)	(segid 3A4 and resid 331 and name CB)	10.65	0.34	0.35
	assign (segid 3A4 and resid 328 and name CB)	(segid 3A4 and resid 332 and name CA)	13.61	0.32	0.32
20	assign (segid 3A4 and resid 328 and name CB)	(segid 3A4 and resid 333 and name CA)	12.73	0.29	0.29
	assign (segid 3A4 and resid 328 and name CB)	(segid 3A4 and resid 335 and name CA)	10.68	0.33	0.33
	assign (segid 3A4 and resid 328 and name CB)	(segid 3A4 and resid 336 and name C)	6.74	0.36	0.35
	assign (segid 3A4 and resid 328 and name CB)	(segid 3A4 and resid 336 and name CA)	7.03	0.39	0.39
	assign (segid 3A4 and resid 328 and name CB)	(segid 3A4 and resid 336 and name CB)	6.87	0.51	0.51
25	assign (segid 3A4 and resid 328 and name CB)	(segid 3A4 and resid 337 and name C)	4.98	0.09	0.10
	assign (segid 3A4 and resid 328 and name CB)	(segid 3A4 and resid 337 and name CA)	6.23	0.11	0.10
	assign (segid 3A4 and resid 328 and name CB)	(segid 3A4 and resid 337 and name CB)	6.87	0.15	0.15
	assign (segid 3A4 and resid 328 and name CB)	(segid 3A4 and resid 337 and name N)	6.14	0.14	0.14
	assign (segid 3A4 and resid 328 and name CB)	(segid 3A4 and resid 337 and name O)	3.95	0.11	0.11
30	assign (segid 3A4 and resid 328 and name CB)	(segid 3A4 and resid 338 and name C)	5.04	0.13	0.14
	assign (segid 3A4 and resid 328 and name CB)	(segid 3A4 and resid 338 and name CA)	4.73	0.15	0.15
	assign (segid 3A4 and resid 328 and name CB)	(segid 3A4 and resid 338 and name CB)	5.69	0.29	0.29
	assign (segid 3A4 and resid 328 and name CB)	(segid 3A4 and resid 338 and name N)	5.34	0.11	0.10
	assign (segid 3A4 and resid 328 and name CB)	(segid 3A4 and resid 338 and name O)	6.04	0.23	0.24
35	assign (segid 3A4 and resid 328 and name CB)	(segid 3A4 and resid 339 and name C)	6.83	0.23	0.24
	assign (segid 3A4 and resid 328 and name CB)	(segid 3A4 and resid 339 and name CA)	5.42	0.26	0.26
	assign (segid 3A4 and resid 328 and name CB)	(segid 3A4 and resid 339 and name CB)	5.40	0.30	0.30
	assign (segid 3A4 and resid 328 and name CB)	(segid 3A4 and resid 339 and name N)	4.59	0.13	0.12
	assign (segid 3A4 and resid 328 and name CB)	(segid 3A4 and resid 339 and name O)	7.25	0.21	0.20
40	assign (segid 3A4 and resid 328 and name CB)	(segid 3A4 and resid 340 and name CA)	9.13	0.26	0.26
	assign (segid 3A4 and resid 328 and name CB)	(segid 3A4 and resid 340 and name N)	7.75	0.28	0.27
	assign (segid 3A4 and resid 328 and name CB)	(segid 3A4 and resid 341 and name CA)	9.77	0.18	0.17
	assign (segid 3A4 and resid 328 and name CB)	(segid 3A4 and resid 341 and name CB)	9.06	0.18	0.18
	assign (segid 3A4 and resid 328 and name CB)	(segid 3A4 and resid 342 and name CA)	12.93	0.23	0.23
45	assign (segid 3A4 and resid 328 and name CB)	(segid 3A4 and resid 343 and name CA)	13.83	0.47	0.47
	assign (segid 3A4 and resid 328 and name CB)	(segid 3A4 and resid 343 and name CB)	13.02	0.57	0.57
	assign (segid 3A4 and resid 328 and name CB)	(segid 3A4 and resid 344 and name CA)	17.51	0.52	0.52
	assign (segid 3A4 and resid 328 and name CB)	(segid 3A4 and resid 344 and name CB)	18.43	0.48	0.47
	assign (segid 3A4 and resid 328 and name N)	(segid 3A4 and resid 328 and name C)	2.39	0.04	0.04
50	assign (segid 3A4 and resid 328 and name N)	(segid 3A4 and resid 328 and name CA)	1.46	0.01	0.01
	assign (segid 3A4 and resid 328 and name N)	(segid 3A4 and resid 328 and name CB)	2.46	0.02	0.02
	assign (segid 3A4 and resid 328 and name N)	(segid 3A4 and resid 328 and name O)	2.70	0.09	0.09
	assign (segid 3A4 and resid 328 and name N)	(segid 3A4 and resid 329 and name C)	5.91	0.03	0.04
	assign (segid 3A4 and resid 328 and name N)	(segid 3A4 and resid 329 and name CA)	4.71	0.04	0.03
55	assign (segid 3A4 and resid 328 and name N)	(segid 3A4 and resid 329 and name CB)	5.09	0.16	0.16
	assign (segid 3A4 and resid 328 and name N)	(segid 3A4 and resid 329 and name N)	3.51	0.03	0.03
	assign (segid 3A4 and resid 328 and name N)	(segid 3A4 and resid 329 and name O)	6.14	0.06	0.05
	assign (segid 3A4 and resid 328 and name N)	(segid 3A4 and resid 330 and name N)	6.94	0.09	0.09
	assign (segid 3A4 and resid 328 and name N)	(segid 3A4 and resid 337 and name C)	5.52	0.18	0.19
60	assign (segid 3A4 and resid 328 and name N)	(segid 3A4 and resid 337 and name CA)	6.78	0.17	0.17
	assign (segid 3A4 and resid 328 and name N)	(segid 3A4 and resid 337 and name CB)	6.96	0.20	0.21
	assign (segid 3A4 and resid 328 and name N)	(segid 3A4 and resid 337 and name N)	7.08	0.14	0.13
	assign (segid 3A4 and resid 328 and name N)	(segid 3A4 and resid 337 and name O)	4.50	0.18	0.19
	assign (segid 3A4 and resid 328 and name N)	(segid 3A4 and resid 338 and name C)	4.74	0.16	0.16
65	assign (segid 3A4 and resid 328 and name N)	(segid 3A4 and resid 338 and name CA)	5.17	0.28	0.28
	assign (segid 3A4 and resid 328 and name N)	(segid 3A4 and resid 338 and name CB)	6.34	0.36	0.36
	assign (segid 3A4 and resid 328 and name N)	(segid 3A4 and resid 338 and name N)	5.85	0.23	0.23
	assign (segid 3A4 and resid 328 and name N)	(segid 3A4 and resid 338 and name O)	5.46	0.17	0.18
	assign (segid 3A4 and resid 328 and name N)	(segid 3A4 and resid 339 and name C)	5.70	0.15	0.16
70	assign (segid 3A4 and resid 328 and name N)	(segid 3A4 and resid 339 and name CA)	4.20	0.13	0.14
	assign (segid 3A4 and resid 328 and name N)	(segid 3A4 and resid 339 and name CB)	4.12	0.17	0.17
	assign (segid 3A4 and resid 328 and name N)	(segid 3A4 and resid 339 and name N)	4.01	0.16	0.16
	assign (segid 3A4 and resid 328 and name N)	(segid 3A4 and resid 339 and name O)	6.47	0.15	0.15
	assign (segid 3A4 and resid 328 and name N)	(segid 3A4 and resid 340 and name CA)	7.77	0.22	0.21
75	assign (segid 3A4 and resid 328 and name N)	(segid 3A4 and resid 340 and name N)	6.32	0.21	0.22
	assign (segid 3A4 and resid 328 and name O)	(segid 3A4 and resid 328 and name CB)	3.16	0.11	0.11
	assign (segid 3A4 and resid 328 and name O)	(segid 3A4 and resid 329 and name C)	4.12	0.05	0.06
	assign (segid 3A4 and resid 328 and name O)	(segid 3A4 and resid 329 and name CA)	2.75	0.01	0.02
	assign (segid 3A4 and resid 328 and name O)	(segid 3A4 and resid 329 and name CB)	3.37	0.16	0.17
80	assign (segid 3A4 and resid 328 and name O)	(segid 3A4 and resid 329 and name N)	2.26	0.02	0.01
	assign (segid 3A4 and resid 328 and name O)	(segid 3A4 and resid 329 and name O)	1.80	0.07	0.07
	assign (segid 3A4 and resid 328 and name O)	(segid 3A4 and resid 330 and name C)	7.17	0.10	0.10
	assign (segid 3A4 and resid 328 and name O)	(segid 3A4 and resid 330 and name CA)	6.23	0.14	0.13

	assign (segid 3A4 and resid 328 and name O)	(segid 3A4 and resid 330 and name CB)	6.77	0.19	0.19
	assign (segid 3A4 and resid 328 and name O)	(segid 3A4 and resid 330 and name N)	4.85	0.14	0.14
	assign (segid 3A4 and resid 328 and name O)	(segid 3A4 and resid 337 and name C)	6.00	0.13	0.12
	assign (segid 3A4 and resid 328 and name O)	(segid 3A4 and resid 337 and name CA)	6.82	0.13	0.13
5	assign (segid 3A4 and resid 328 and name O)	(segid 3A4 and resid 337 and name CB)	6.83	0.19	0.18
	assign (segid 3A4 and resid 328 and name O)	(segid 3A4 and resid 337 and name N)	6.67	0.14	0.13
	assign (segid 3A4 and resid 328 and name O)	(segid 3A4 and resid 337 and name O)	4.83	0.15	0.14
	assign (segid 3A4 and resid 328 and name O)	(segid 3A4 and resid 338 and name C)	6.56	0.08	0.08
	assign (segid 3A4 and resid 328 and name O)	(segid 3A4 and resid 338 and name CA)	6.64	0.20	0.19
10	assign (segid 3A4 and resid 328 and name O)	(segid 3A4 and resid 338 and name N)	6.81	0.15	0.15
	assign (segid 3A4 and resid 328 and name O)	(segid 3A4 and resid 338 and name O)	7.14	0.19	0.19
	assign (segid 3A4 and resid 328 and name O)	(segid 3A4 and resid 339 and name CA)	6.61	0.16	0.16
	assign (segid 3A4 and resid 328 and name O)	(segid 3A4 and resid 339 and name CB)	6.75	0.19	0.19
	assign (segid 3A4 and resid 328 and name O)	(segid 3A4 and resid 339 and name N)	6.22	0.07	0.07
15	assign (segid 3A4 and resid 329 and name C)	(segid 3A4 and resid 329 and name CB)	2.52	0.05	0.04
	assign (segid 3A4 and resid 329 and name C)	(segid 3A4 and resid 329 and name O)	1.23	0.01	0.01
	assign (segid 3A4 and resid 329 and name C)	(segid 3A4 and resid 330 and name C)	3.36	0.06	0.06
	assign (segid 3A4 and resid 329 and name C)	(segid 3A4 and resid 330 and name CA)	2.41	0.01	0.01
	assign (segid 3A4 and resid 329 and name C)	(segid 3A4 and resid 330 and name CB)	3.49	0.10	0.11
20	assign (segid 3A4 and resid 329 and name C)	(segid 3A4 and resid 330 and name N)	1.32	0.01	0.01
	assign (segid 3A4 and resid 329 and name C)	(segid 3A4 and resid 330 and name O)	4.02	0.16	0.17
	assign (segid 3A4 and resid 329 and name C)	(segid 3A4 and resid 331 and name C)	6.31	0.20	0.21
	assign (segid 3A4 and resid 329 and name C)	(segid 3A4 and resid 331 and name CA)	5.21	0.24	0.23
	assign (segid 3A4 and resid 329 and name C)	(segid 3A4 and resid 331 and name CB)	5.54	0.33	0.33
25	assign (segid 3A4 and resid 329 and name C)	(segid 3A4 and resid 331 and name N)	3.94	0.24	0.25
	assign (segid 3A4 and resid 329 and name C)	(segid 3A4 and resid 331 and name O)	6.52	0.20	0.21
	assign (segid 3A4 and resid 329 and name C)	(segid 3A4 and resid 332 and name N)	7.26	0.22	0.22
	assign (segid 3A4 and resid 329 and name C)	(segid 3A4 and resid 335 and name C)	5.67	0.38	0.38
	assign (segid 3A4 and resid 329 and name C)	(segid 3A4 and resid 335 and name CA)	6.90	0.23	0.23
30	assign (segid 3A4 and resid 329 and name C)	(segid 3A4 and resid 335 and name N)	7.07	0.23	0.24
	assign (segid 3A4 and resid 329 and name C)	(segid 3A4 and resid 335 and name O)	5.24	0.99	0.99
	assign (segid 3A4 and resid 329 and name C)	(segid 3A4 and resid 336 and name C)	4.75	0.11	0.10
	assign (segid 3A4 and resid 329 and name C)	(segid 3A4 and resid 336 and name CA)	4.52	0.18	0.19
	assign (segid 3A4 and resid 329 and name C)	(segid 3A4 and resid 336 and name CB)	5.36	0.19	0.18
35	assign (segid 3A4 and resid 329 and name C)	(segid 3A4 and resid 336 and name N)	5.35	0.25	0.25
	assign (segid 3A4 and resid 329 and name C)	(segid 3A4 and resid 336 and name O)	5.93	0.09	0.10
	assign (segid 3A4 and resid 329 and name C)	(segid 3A4 and resid 337 and name C)	4.80	0.08	0.07
	assign (segid 3A4 and resid 329 and name C)	(segid 3A4 and resid 337 and name CA)	4.65	0.08	0.07
	assign (segid 3A4 and resid 329 and name C)	(segid 3A4 and resid 337 and name CB)	4.52	0.21	0.21
40	assign (segid 3A4 and resid 329 and name C)	(segid 3A4 and resid 337 and name N)	3.89	0.05	0.06
	assign (segid 3A4 and resid 329 and name C)	(segid 3A4 and resid 337 and name O)	4.06	0.10	0.09
	assign (segid 3A4 and resid 329 and name C)	(segid 3A4 and resid 338 and name C)	7.21	0.12	0.13
	assign (segid 3A4 and resid 329 and name C)	(segid 3A4 and resid 338 and name CA)	6.76	0.09	0.10
	assign (segid 3A4 and resid 329 and name C)	(segid 3A4 and resid 338 and name N)	6.07	0.09	0.08
45	assign (segid 3A4 and resid 329 and name C)	(segid 3A4 and resid 338 and name O)	7.50	0.27	0.26
	assign (segid 3A4 and resid 329 and name C)	(segid 3A4 and resid 339 and name N)	7.63	0.11	0.11
	assign (segid 3A4 and resid 329 and name CA)	(segid 3A4 and resid 329 and name C)	1.52	0.01	0.00
	assign (segid 3A4 and resid 329 and name CA)	(segid 3A4 and resid 329 and name CB)	1.55	0.02	0.02
	assign (segid 3A4 and resid 329 and name CA)	(segid 3A4 and resid 329 and name O)	2.39	0.01	0.01
50	assign (segid 3A4 and resid 329 and name CA)	(segid 3A4 and resid 330 and name C)	4.58	0.04	0.05
	assign (segid 3A4 and resid 329 and name CA)	(segid 3A4 and resid 330 and name CA)	3.77	0.01	0.02
	assign (segid 3A4 and resid 329 and name CA)	(segid 3A4 and resid 330 and name CB)	4.69	0.08	0.08
	assign (segid 3A4 and resid 329 and name CA)	(segid 3A4 and resid 330 and name N)	2.41	0.03	0.03
	assign (segid 3A4 and resid 329 and name CA)	(segid 3A4 and resid 330 and name O)	5.00	0.25	0.24
55	assign (segid 3A4 and resid 329 and name CA)	(segid 3A4 and resid 331 and name C)	7.59	0.23	0.22
	assign (segid 3A4 and resid 329 and name CA)	(segid 3A4 and resid 331 and name CA)	6.35	0.26	0.27
	assign (segid 3A4 and resid 329 and name CA)	(segid 3A4 and resid 331 and name CB)	6.55	0.38	0.38
	assign (segid 3A4 and resid 329 and name CA)	(segid 3A4 and resid 331 and name N)	5.23	0.27	0.27
	assign (segid 3A4 and resid 329 and name CA)	(segid 3A4 and resid 332 and name CA)	9.75	0.22	0.22
60	assign (segid 3A4 and resid 329 and name CA)	(segid 3A4 and resid 333 and name CA)	9.77	0.49	0.49
	assign (segid 3A4 and resid 329 and name CA)	(segid 3A4 and resid 335 and name C)	7.12	0.37	0.37
	assign (segid 3A4 and resid 329 and name CA)	(segid 3A4 and resid 335 and name CA)	8.38	0.24	0.23
	assign (segid 3A4 and resid 329 and name CA)	(segid 3A4 and resid 336 and name C)	5.78	0.14	0.14
	assign (segid 3A4 and resid 329 and name CA)	(segid 3A4 and resid 336 and name CA)	5.77	0.20	0.19
65	assign (segid 3A4 and resid 329 and name CA)	(segid 3A4 and resid 336 and name CB)	6.47	0.22	0.21
	assign (segid 3A4 and resid 329 and name CA)	(segid 3A4 and resid 336 and name N)	6.74	0.25	0.24
	assign (segid 3A4 and resid 329 and name CA)	(segid 3A4 and resid 336 and name O)	6.89	0.14	0.14
	assign (segid 3A4 and resid 329 and name CA)	(segid 3A4 and resid 337 and name C)	4.97	0.05	0.06
	assign (segid 3A4 and resid 329 and name CA)	(segid 3A4 and resid 337 and name CA)	5.21	0.08	0.07
70	assign (segid 3A4 and resid 329 and name CA)	(segid 3A4 and resid 337 and name CB)	4.99	0.17	0.17
	assign (segid 3A4 and resid 329 and name CA)	(segid 3A4 and resid 337 and name N)	4.79	0.08	0.08
	assign (segid 3A4 and resid 329 and name CA)	(segid 3A4 and resid 337 and name O)	4.01	0.08	0.08
	assign (segid 3A4 and resid 329 and name CA)	(segid 3A4 and resid 338 and name C)	6.77	0.08	0.09
	assign (segid 3A4 and resid 329 and name CA)	(segid 3A4 and resid 338 and name CA)	6.58	0.12	0.12
75	assign (segid 3A4 and resid 329 and name CA)	(segid 3A4 and resid 338 and name CB)	7.97	0.16	0.16
	assign (segid 3A4 and resid 329 and name CA)	(segid 3A4 and resid 338 and name N)	6.15	0.09	0.09
	assign (segid 3A4 and resid 329 and name CA)	(segid 3A4 and resid 338 and name O)	7.09	0.25	0.26
	assign (segid 3A4 and resid 329 and name CA)	(segid 3A4 and resid 339 and name CA)	7.61	0.19	0.18
	assign (segid 3A4 and resid 329 and name CA)	(segid 3A4 and resid 339 and name CB)	8.24	0.19	0.20
80	assign (segid 3A4 and resid 329 and name CA)	(segid 3A4 and resid 339 and name N)	6.97	0.07	0.07
	assign (segid 3A4 and resid 329 and name CA)	(segid 3A4 and resid 340 and name CA)	10.52	0.26	0.25
	assign (segid 3A4 and resid 329 and name CA)	(segid 3A4 and resid 341 and name CA)	10.04	0.19	0.19
	assign (segid 3A4 and resid 329 and name CA)	(segid 3A4 and resid 341 and name CB)	9.11	0.18	0.17

	assign (segid 3A4 and resid 329 and name CA)	(segid 3A4 and resid 342 and name CA)	12.16	0.38	0.38
	assign (segid 3A4 and resid 329 and name CA)	(segid 3A4 and resid 343 and name CA)	11.79	0.65	0.65
	assign (segid 3A4 and resid 329 and name CA)	(segid 3A4 and resid 343 and name CB)	10.63	0.73	0.73
	assign (segid 3A4 and resid 329 and name CA)	(segid 3A4 and resid 344 and name CA)	15.10	0.76	0.76
	assign (segid 3A4 and resid 329 and name CA)	(segid 3A4 and resid 344 and name CB)	16.20	0.70	0.70
5	assign (segid 3A4 and resid 329 and name CA)	(segid 3A4 and resid 345 and name CA)	15.67	1.02	1.02
	assign (segid 3A4 and resid 329 and name CA)	(segid 3A4 and resid 345 and name CB)	15.30	1.11	1.11
	assign (segid 3A4 and resid 329 and name CA)	(segid 3A4 and resid 387 and name CA)	17.90	0.98	0.98
	assign (segid 3A4 and resid 329 and name CB)	(segid 3A4 and resid 330 and name C)	4.88	0.12	0.13
	assign (segid 3A4 and resid 329 and name CB)	(segid 3A4 and resid 330 and name CA)	4.52	0.14	0.14
10	assign (segid 3A4 and resid 329 and name CB)	(segid 3A4 and resid 330 and name CB)	5.66	0.20	0.19
	assign (segid 3A4 and resid 329 and name CB)	(segid 3A4 and resid 330 and name N)	3.23	0.16	0.16
	assign (segid 3A4 and resid 329 and name CB)	(segid 3A4 and resid 330 and name O)	5.12	0.39	0.40
	assign (segid 3A4 and resid 329 and name CB)	(segid 3A4 and resid 331 and name C)	7.58	0.26	0.26
	assign (segid 3A4 and resid 329 and name CB)	(segid 3A4 and resid 331 and name CA)	6.20	0.29	0.29
15	assign (segid 3A4 and resid 329 and name CB)	(segid 3A4 and resid 331 and name CB)	6.14	0.44	0.44
	assign (segid 3A4 and resid 329 and name CB)	(segid 3A4 and resid 331 and name N)	5.37	0.30	0.29
	assign (segid 3A4 and resid 329 and name CB)	(segid 3A4 and resid 332 and name CA)	9.81	0.25	0.24
	assign (segid 3A4 and resid 329 and name CB)	(segid 3A4 and resid 333 and name CA)	10.35	0.53	0.53
	assign (segid 3A4 and resid 329 and name CB)	(segid 3A4 and resid 335 and name CA)	8.99	0.26	0.26
20	assign (segid 3A4 and resid 329 and name CB)	(segid 3A4 and resid 336 and name C)	6.57	0.21	0.21
	assign (segid 3A4 and resid 329 and name CB)	(segid 3A4 and resid 336 and name CA)	6.75	0.26	0.25
	assign (segid 3A4 and resid 329 and name CB)	(segid 3A4 and resid 336 and name CB)	7.65	0.26	0.25
	assign (segid 3A4 and resid 329 and name CB)	(segid 3A4 and resid 337 and name C)	5.45	0.14	0.14
	assign (segid 3A4 and resid 329 and name CB)	(segid 3A4 and resid 337 and name CA)	5.56	0.14	0.14
25	assign (segid 3A4 and resid 329 and name CB)	(segid 3A4 and resid 337 and name CB)	4.92	0.13	0.14
	assign (segid 3A4 and resid 329 and name CB)	(segid 3A4 and resid 337 and name N)	5.43	0.19	0.19
	assign (segid 3A4 and resid 329 and name CB)	(segid 3A4 and resid 337 and name O)	4.61	0.19	0.19
	assign (segid 3A4 and resid 329 and name CB)	(segid 3A4 and resid 338 and name C)	7.00	0.10	0.10
	assign (segid 3A4 and resid 329 and name CB)	(segid 3A4 and resid 338 and name CA)	7.07	0.16	0.16
30	assign (segid 3A4 and resid 329 and name CB)	(segid 3A4 and resid 338 and name CB)	8.53	0.17	0.16
	assign (segid 3A4 and resid 329 and name CB)	(segid 3A4 and resid 338 and name N)	6.60	0.15	0.15
	assign (segid 3A4 and resid 329 and name CB)	(segid 3A4 and resid 338 and name O)	7.08	0.22	0.23
	assign (segid 3A4 and resid 329 and name CB)	(segid 3A4 and resid 339 and name C)	7.62	0.18	0.19
	assign (segid 3A4 and resid 329 and name CB)	(segid 3A4 and resid 339 and name CB)	8.36	0.16	0.17
35	assign (segid 3A4 and resid 329 and name CB)	(segid 3A4 and resid 339 and name N)	7.22	0.14	0.14
	assign (segid 3A4 and resid 329 and name CB)	(segid 3A4 and resid 340 and name CA)	10.16	0.32	0.33
	assign (segid 3A4 and resid 329 and name CB)	(segid 3A4 and resid 341 and name CA)	9.66	0.29	0.29
	assign (segid 3A4 and resid 329 and name CB)	(segid 3A4 and resid 341 and name CB)	8.83	0.27	0.28
40	assign (segid 3A4 and resid 329 and name CB)	(segid 3A4 and resid 342 and name CA)	11.40	0.46	0.47
	assign (segid 3A4 and resid 329 and name CB)	(segid 3A4 and resid 343 and name CA)	10.85	0.75	0.75
	assign (segid 3A4 and resid 329 and name CB)	(segid 3A4 and resid 343 and name CB)	9.62	0.82	0.82
	assign (segid 3A4 and resid 329 and name CB)	(segid 3A4 and resid 344 and name CA)	14.08	0.86	0.85
	assign (segid 3A4 and resid 329 and name CB)	(segid 3A4 and resid 344 and name CB)	15.25	0.80	0.80
	assign (segid 3A4 and resid 329 and name CB)	(segid 3A4 and resid 345 and name CA)	14.52	1.07	1.08
45	assign (segid 3A4 and resid 329 and name CB)	(segid 3A4 and resid 345 and name CB)	14.07	1.16	1.15
	assign (segid 3A4 and resid 329 and name CB)	(segid 3A4 and resid 346 and name CA)	17.96	1.03	1.04
	assign (segid 3A4 and resid 329 and name CB)	(segid 3A4 and resid 346 and name CB)	18.39	0.95	0.95
	assign (segid 3A4 and resid 329 and name CB)	(segid 3A4 and resid 386 and name CA)	17.73	0.65	0.65
	assign (segid 3A4 and resid 329 and name CB)	(segid 3A4 and resid 387 and name CA)	16.44	0.95	0.94
50	assign (segid 3A4 and resid 329 and name CB)	(segid 3A4 and resid 388 and name CA)	17.60	1.19	1.19
	assign (segid 3A4 and resid 329 and name CB)	(segid 3A4 and resid 388 and name CB)	16.97	1.32	1.33
	assign (segid 3A4 and resid 329 and name CB)	(segid 3A4 and resid 389 and name CB)	17.59	1.10	1.10
	assign (segid 3A4 and resid 329 and name N)	(segid 3A4 and resid 329 and name C)	2.42	0.01	0.02
	assign (segid 3A4 and resid 329 and name N)	(segid 3A4 and resid 329 and name CA)	1.46	0.01	0.00
55	assign (segid 3A4 and resid 329 and name N)	(segid 3A4 and resid 329 and name CB)	2.47	0.02	0.01
	assign (segid 3A4 and resid 329 and name N)	(segid 3A4 and resid 329 and name O)	2.74	0.04	0.04
	assign (segid 3A4 and resid 329 and name N)	(segid 3A4 and resid 330 and name C)	5.75	0.04	0.05
	assign (segid 3A4 and resid 329 and name N)	(segid 3A4 and resid 330 and name CA)	4.76	0.04	0.04
	assign (segid 3A4 and resid 329 and name N)	(segid 3A4 and resid 330 and name CB)	5.59	0.05	0.05
60	assign (segid 3A4 and resid 329 and name N)	(segid 3A4 and resid 330 and name N)	3.54	0.06	0.06
	assign (segid 3A4 and resid 329 and name N)	(segid 3A4 and resid 330 and name O)	6.30	0.21	0.20
	assign (segid 3A4 and resid 329 and name N)	(segid 3A4 and resid 331 and name CA)	7.46	0.22	0.22
	assign (segid 3A4 and resid 329 and name N)	(segid 3A4 and resid 331 and name N)	6.28	0.23	0.23
	assign (segid 3A4 and resid 329 and name N)	(segid 3A4 and resid 335 and name C)	7.40	0.35	0.35
65	assign (segid 3A4 and resid 329 and name N)	(segid 3A4 and resid 336 and name C)	5.46	0.19	0.19
	assign (segid 3A4 and resid 329 and name N)	(segid 3A4 and resid 336 and name CA)	5.69	0.23	0.22
	assign (segid 3A4 and resid 329 and name N)	(segid 3A4 and resid 336 and name CB)	6.21	0.27	0.27
	assign (segid 3A4 and resid 329 and name N)	(segid 3A4 and resid 336 and name N)	6.86	0.24	0.25
	assign (segid 3A4 and resid 329 and name N)	(segid 3A4 and resid 336 and name O)	6.44	0.22	0.22
70	assign (segid 3A4 and resid 329 and name N)	(segid 3A4 and resid 337 and name C)	4.06	0.09	0.09
	assign (segid 3A4 and resid 329 and name N)	(segid 3A4 and resid 337 and name CA)	4.68	0.13	0.12
	assign (segid 3A4 and resid 329 and name N)	(segid 3A4 and resid 337 and name CB)	4.72	0.21	0.22
	assign (segid 3A4 and resid 329 and name N)	(segid 3A4 and resid 337 and name N)	4.47	0.11	0.10
	assign (segid 3A4 and resid 329 and name N)	(segid 3A4 and resid 337 and name O)	2.95	0.10	0.09
75	assign (segid 3A4 and resid 329 and name N)	(segid 3A4 and resid 338 and name C)	5.51	0.11	0.10
	assign (segid 3A4 and resid 329 and name N)	(segid 3A4 and resid 338 and name CA)	5.31	0.13	0.14
	assign (segid 3A4 and resid 329 and name N)	(segid 3A4 and resid 338 and name CB)	6.69	0.19	0.19
	assign (segid 3A4 and resid 329 and name N)	(segid 3A4 and resid 338 and name N)	5.10	0.11	0.10
	assign (segid 3A4 and resid 329 and name N)	(segid 3A4 and resid 338 and name O)	5.97	0.28	0.28
80	assign (segid 3A4 and resid 329 and name N)	(segid 3A4 and resid 338 and name C)	7.61	0.21	0.20
	assign (segid 3A4 and resid 329 and name N)	(segid 3A4 and resid 339 and name CA)	6.33	0.21	0.21
	assign (segid 3A4 and resid 329 and name N)	(segid 3A4 and resid 339 and name CB)	6.93	0.22	0.22

	assign (segid 3A4 and resid 329 and name N)	(segid 3A4 and resid 339 and name N)	5.62	0.08	0.08
	assign (segid 3A4 and resid 329 and name O)	(segid 3A4 and resid 329 and name CB)	3.23	0.14	0.14
	assign (segid 3A4 and resid 329 and name O)	(segid 3A4 and resid 330 and name C)	3.70	0.11	0.10
	assign (segid 3A4 and resid 329 and name O)	(segid 3A4 and resid 330 and name CA)	2.74	0.05	0.04
	assign (segid 3A4 and resid 329 and name O)	(segid 3A4 and resid 330 and name CB)	3.89	0.18	0.18
5	assign (segid 3A4 and resid 329 and name O)	(segid 3A4 and resid 330 and name N)	2.24	0.02	0.03
	assign (segid 3A4 and resid 329 and name O)	(segid 3A4 and resid 330 and name O)	4.60	0.10	0.11
	assign (segid 3A4 and resid 329 and name O)	(segid 3A4 and resid 331 and name C)	6.20	0.29	0.28
	assign (segid 3A4 and resid 329 and name O)	(segid 3A4 and resid 331 and name CA)	5.22	0.31	0.31
	assign (segid 3A4 and resid 329 and name O)	(segid 3A4 and resid 331 and name CB)	5.39	0.45	0.44
10	assign (segid 3A4 and resid 329 and name O)	(segid 3A4 and resid 331 and name N)	3.94	0.29	0.28
	assign (segid 3A4 and resid 329 and name O)	(segid 3A4 and resid 331 and name O)	6.18	0.30	0.31
	assign (segid 3A4 and resid 329 and name O)	(segid 3A4 and resid 332 and name N)	7.28	0.28	0.27
	assign (segid 3A4 and resid 329 and name O)	(segid 3A4 and resid 335 and name C)	4.83	0.36	0.37
	assign (segid 3A4 and resid 329 and name O)	(segid 3A4 and resid 335 and name CA)	6.13	0.25	0.24
15	assign (segid 3A4 and resid 329 and name O)	(segid 3A4 and resid 335 and name N)	6.51	0.24	0.24
	assign (segid 3A4 and resid 329 and name O)	(segid 3A4 and resid 335 and name O)	4.46	0.89	0.90
	assign (segid 3A4 and resid 329 and name O)	(segid 3A4 and resid 336 and name C)	3.60	0.12	0.11
	assign (segid 3A4 and resid 329 and name O)	(segid 3A4 and resid 336 and name CA)	3.55	0.21	0.21
	assign (segid 3A4 and resid 329 and name O)	(segid 3A4 and resid 336 and name CB)	4.52	0.17	0.18
20	assign (segid 3A4 and resid 329 and name O)	(segid 3A4 and resid 336 and name N)	4.44	0.27	0.27
	assign (segid 3A4 and resid 329 and name O)	(segid 3A4 and resid 336 and name O)	4.78	0.10	0.10
	assign (segid 3A4 and resid 329 and name O)	(segid 3A4 and resid 337 and name C)	3.87	0.11	0.10
	assign (segid 3A4 and resid 329 and name O)	(segid 3A4 and resid 337 and name CA)	3.54	0.10	0.11
	assign (segid 3A4 and resid 329 and name O)	(segid 3A4 and resid 337 and name CB)	3.58	0.23	0.23
25	assign (segid 3A4 and resid 329 and name O)	(segid 3A4 and resid 337 and name N)	2.71	0.06	0.07
	assign (segid 3A4 and resid 329 and name O)	(segid 3A4 and resid 337 and name O)	3.33	0.14	0.15
	assign (segid 3A4 and resid 329 and name O)	(segid 3A4 and resid 338 and name C)	6.60	0.14	0.15
	assign (segid 3A4 and resid 329 and name O)	(segid 3A4 and resid 338 and name CA)	6.01	0.10	0.10
	assign (segid 3A4 and resid 329 and name O)	(segid 3A4 and resid 338 and name CB)	7.25	0.12	0.11
30	assign (segid 3A4 and resid 329 and name O)	(segid 3A4 and resid 338 and name N)	5.15	0.09	0.09
	assign (segid 3A4 and resid 329 and name O)	(segid 3A4 and resid 338 and name O)	6.85	0.26	0.26
	assign (segid 3A4 and resid 329 and name O)	(segid 3A4 and resid 339 and name N)	7.20	0.13	0.12
	assign (segid 3A4 and resid 329 and name O)	(segid 3A4 and resid 32 and name CB)	2.51	0.03	0.03
	assign (segid 3A4 and resid 32 and name C)	(segid 3A4 and resid 32 and name O)	1.24	0.02	0.01
35	assign (segid 3A4 and resid 32 and name C)	(segid 3A4 and resid 33 and name C)	3.25	0.09	0.10
	assign (segid 3A4 and resid 32 and name C)	(segid 3A4 and resid 33 and name CA)	2.43	0.01	0.02
	assign (segid 3A4 and resid 32 and name C)	(segid 3A4 and resid 33 and name CB)	3.62	0.03	0.03
	assign (segid 3A4 and resid 32 and name C)	(segid 3A4 and resid 33 and name N)	1.32	0.03	0.02
	assign (segid 3A4 and resid 32 and name C)	(segid 3A4 and resid 33 and name O)	3.78	0.15	0.16
40	assign (segid 3A4 and resid 32 and name C)	(segid 3A4 and resid 342 and name O)	7.58	0.11	0.10
	assign (segid 3A4 and resid 32 and name C)	(segid 3A4 and resid 343 and name C)	6.38	0.15	0.14
	assign (segid 3A4 and resid 32 and name C)	(segid 3A4 and resid 343 and name CA)	6.48	0.17	0.17
	assign (segid 3A4 and resid 32 and name C)	(segid 3A4 and resid 343 and name CB)	6.62	0.26	0.26
	assign (segid 3A4 and resid 32 and name C)	(segid 3A4 and resid 343 and name O)	7.40	0.21	0.21
45	assign (segid 3A4 and resid 32 and name C)	(segid 3A4 and resid 344 and name C)	4.96	0.08	0.08
	assign (segid 3A4 and resid 32 and name C)	(segid 3A4 and resid 344 and name CA)	5.64	0.11	0.11
	assign (segid 3A4 and resid 32 and name C)	(segid 3A4 and resid 344 and name CB)	5.71	0.29	0.28
	assign (segid 3A4 and resid 32 and name C)	(segid 3A4 and resid 344 and name N)	5.36	0.09	0.09
	assign (segid 3A4 and resid 32 and name C)	(segid 3A4 and resid 344 and name O)	3.78	0.10	0.09
50	assign (segid 3A4 and resid 32 and name C)	(segid 3A4 and resid 345 and name C)	6.50	0.19	0.19
	assign (segid 3A4 and resid 32 and name C)	(segid 3A4 and resid 345 and name CA)	5.90	0.16	0.15
	assign (segid 3A4 and resid 32 and name C)	(segid 3A4 and resid 345 and name CB)	7.03	0.24	0.23
	assign (segid 3A4 and resid 32 and name C)	(segid 3A4 and resid 345 and name N)	5.88	0.12	0.12
	assign (segid 3A4 and resid 32 and name C)	(segid 3A4 and resid 346 and name CA)	6.93	0.36	0.35
55	assign (segid 3A4 and resid 32 and name C)	(segid 3A4 and resid 346 and name CB)	6.38	0.44	0.45
	assign (segid 3A4 and resid 32 and name C)	(segid 3A4 and resid 346 and name N)	5.99	0.24	0.25
	assign (segid 3A4 and resid 32 and name C)	(segid 3A4 and resid 34 and name C)	6.43	0.22	0.23
	assign (segid 3A4 and resid 32 and name C)	(segid 3A4 and resid 34 and name CA)	5.11	0.21	0.21
	assign (segid 3A4 and resid 32 and name C)	(segid 3A4 and resid 34 and name CB)	5.40	0.21	0.21
60	assign (segid 3A4 and resid 32 and name C)	(segid 3A4 and resid 34 and name N)	3.95	0.21	0.20
	assign (segid 3A4 and resid 32 and name C)	(segid 3A4 and resid 34 and name O)	7.45	0.22	0.21
	assign (segid 3A4 and resid 32 and name C)	(segid 3A4 and resid 35 and name N)	6.72	0.25	0.25
	assign (segid 3A4 and resid 32 and name C)	(segid 3A4 and resid 38 and name CB)	7.33	0.30	0.31
	assign (segid 3A4 and resid 32 and name CA)	(segid 3A4 and resid 317 and name CA)	16.58	0.37	0.38
65	assign (segid 3A4 and resid 32 and name CA)	(segid 3A4 and resid 318 and name CA)	17.33	0.73	0.73
	assign (segid 3A4 and resid 32 and name CA)	(segid 3A4 and resid 318 and name CB)	18.67	0.67	0.67
	assign (segid 3A4 and resid 32 and name CA)	(segid 3A4 and resid 319 and name CA)	14.81	0.59	0.59
	assign (segid 3A4 and resid 32 and name CA)	(segid 3A4 and resid 319 and name CB)	15.21	0.62	0.62
	assign (segid 3A4 and resid 32 and name CA)	(segid 3A4 and resid 322 and name CA)	9.41	0.45	0.45
70	assign (segid 3A4 and resid 32 and name CA)	(segid 3A4 and resid 323 and name CA)	10.39	0.14	0.14
	assign (segid 3A4 and resid 32 and name CA)	(segid 3A4 and resid 323 and name CB)	10.16	0.27	0.28
	assign (segid 3A4 and resid 32 and name CA)	(segid 3A4 and resid 324 and name CA)	11.75	0.32	0.32
	assign (segid 3A4 and resid 32 and name CA)	(segid 3A4 and resid 324 and name CB)	12.91	0.39	0.40
	assign (segid 3A4 and resid 32 and name CA)	(segid 3A4 and resid 325 and name CA)	12.80	0.30	0.31
75	assign (segid 3A4 and resid 32 and name CA)	(segid 3A4 and resid 325 and name CB)	12.32	0.38	0.38
	assign (segid 3A4 and resid 32 and name CA)	(segid 3A4 and resid 326 and name CA)	16.60	0.29	0.30
	assign (segid 3A4 and resid 32 and name CA)	(segid 3A4 and resid 326 and name CB)	17.42	0.29	0.30
	assign (segid 3A4 and resid 32 and name CA)	(segid 3A4 and resid 327 and name CA)	17.43	0.41	0.41
	assign (segid 3A4 and resid 32 and name CA)	(segid 3A4 and resid 327 and name CB)	18.43	0.47	0.46
80	assign (segid 3A4 and resid 32 and name CA)	(segid 3A4 and resid 328 and name CA)	16.31	0.57	0.57
	assign (segid 3A4 and resid 32 and name CA)	(segid 3A4 and resid 328 and name CB)	17.29	0.61	0.61
	assign (segid 3A4 and resid 32 and name CA)	(segid 3A4 and resid 329 and name CA)	14.75	0.73	0.73

	assign (segid 3A4 and resid 32 and name CA) (segid 3A4 and resid 329 and name CB)	14.08	0.83	0.83
	assign (segid 3A4 and resid 32 and name CA) (segid 3A4 and resid 32 and name C)	1.52	0.00	0.01
	assign (segid 3A4 and resid 32 and name CA) (segid 3A4 and resid 32 and name CB)	1.55	0.03	0.02
	assign (segid 3A4 and resid 32 and name CA) (segid 3A4 and resid 32 and name O)	2.38	0.02	0.03
	assign (segid 3A4 and resid 32 and name CA) (segid 3A4 and resid 330 and name CA)	14.13	0.55	0.55
5	assign (segid 3A4 and resid 32 and name CA) (segid 3A4 and resid 330 and name CB)	15.42	0.54	0.54
	assign (segid 3A4 and resid 32 and name CA) (segid 3A4 and resid 331 and name CA)	11.62	0.55	0.54
	assign (segid 3A4 and resid 32 and name CA) (segid 3A4 and resid 331 and name CB)	10.27	0.54	0.54
	assign (segid 3A4 and resid 32 and name CA) (segid 3A4 and resid 332 and name CA)	12.65	0.65	0.66
	assign (segid 3A4 and resid 32 and name CA) (segid 3A4 and resid 333 and name CA)	14.52	0.94	0.94
10	assign (segid 3A4 and resid 32 and name CA) (segid 3A4 and resid 335 and name CA)	11.81	0.47	0.46
	assign (segid 3A4 and resid 32 and name CA) (segid 3A4 and resid 336 and name CA)	13.14	0.44	0.45
	assign (segid 3A4 and resid 32 and name CA) (segid 3A4 and resid 336 and name CB)	14.46	0.42	0.41
	assign (segid 3A4 and resid 32 and name CA) (segid 3A4 and resid 337 and name CA)	11.37	0.64	0.63
	assign (segid 3A4 and resid 32 and name CA) (segid 3A4 and resid 337 and name CB)	10.49	0.70	0.70
15	assign (segid 3A4 and resid 32 and name CA) (segid 3A4 and resid 338 and name CA)	14.01	0.54	0.53
	assign (segid 3A4 and resid 32 and name CA) (segid 3A4 and resid 338 and name CB)	15.57	0.40	0.40
	assign (segid 3A4 and resid 32 and name CA) (segid 3A4 and resid 339 and name CA)	15.57	0.40	0.40
	assign (segid 3A4 and resid 32 and name CA) (segid 3A4 and resid 339 and name CB)	17.09	0.40	0.40
	assign (segid 3A4 and resid 32 and name CA) (segid 3A4 and resid 33 and name C)	4.50	0.09	0.08
20	assign (segid 3A4 and resid 32 and name CA) (segid 3A4 and resid 33 and name CA)	3.80	0.01	0.02
	assign (segid 3A4 and resid 32 and name CA) (segid 3A4 and resid 33 and name CB)	4.80	0.04	0.03
	assign (segid 3A4 and resid 32 and name CA) (segid 3A4 and resid 33 and name N)	2.42	0.01	0.01
	assign (segid 3A4 and resid 32 and name CA) (segid 3A4 and resid 33 and name O)	4.73	0.18	0.17
	assign (segid 3A4 and resid 32 and name CA) (segid 3A4 and resid 340 and name CA)	14.53	0.22	0.22
25	assign (segid 3A4 and resid 32 and name CA) (segid 3A4 and resid 341 and name CA)	10.97	0.23	0.22
	assign (segid 3A4 and resid 32 and name CA) (segid 3A4 and resid 341 and name CB)	10.37	0.33	0.32
	assign (segid 3A4 and resid 32 and name CA) (segid 3A4 and resid 342 and name C)	7.32	0.14	0.14
	assign (segid 3A4 and resid 32 and name CA) (segid 3A4 and resid 342 and name CA)	8.78	0.13	0.13
	assign (segid 3A4 and resid 32 and name CA) (segid 3A4 and resid 342 and name O)	6.65	0.15	0.15
30	assign (segid 3A4 and resid 32 and name CA) (segid 3A4 and resid 343 and name C)	5.67	0.17	0.17
	assign (segid 3A4 and resid 32 and name CA) (segid 3A4 and resid 343 and name CA)	5.83	0.19	0.20
	assign (segid 3A4 and resid 32 and name CA) (segid 3A4 and resid 343 and name CB)	6.31	0.28	0.28
	assign (segid 3A4 and resid 32 and name CA) (segid 3A4 and resid 343 and name N)	7.04	0.16	0.17
	assign (segid 3A4 and resid 32 and name CA) (segid 3A4 and resid 343 and name O)	6.74	0.20	0.20
35	assign (segid 3A4 and resid 32 and name CA) (segid 3A4 and resid 344 and name C)	4.55	0.13	0.13
	assign (segid 3A4 and resid 32 and name CA) (segid 3A4 and resid 344 and name CA)	4.87	0.15	0.14
	assign (segid 3A4 and resid 32 and name CA) (segid 3A4 and resid 344 and name CB)	4.65	0.30	0.31
	assign (segid 3A4 and resid 32 and name CA) (segid 3A4 and resid 344 and name N)	4.57	0.14	0.13
	assign (segid 3A4 and resid 32 and name CA) (segid 3A4 and resid 344 and name O)	3.51	0.17	0.16
40	assign (segid 3A4 and resid 32 and name CA) (segid 3A4 and resid 345 and name C)	6.61	0.19	0.19
	assign (segid 3A4 and resid 32 and name CA) (segid 3A4 and resid 345 and name CA)	6.05	0.15	0.15
	assign (segid 3A4 and resid 32 and name CA) (segid 3A4 and resid 345 and name CB)	7.30	0.23	0.23
	assign (segid 3A4 and resid 32 and name CA) (segid 3A4 and resid 345 and name N)	5.69	0.15	0.15
	assign (segid 3A4 and resid 32 and name CA) (segid 3A4 and resid 346 and name CA)	7.10	0.32	0.31
45	assign (segid 3A4 and resid 32 and name CA) (segid 3A4 and resid 346 and name CB)	6.57	0.43	0.42
	assign (segid 3A4 and resid 32 and name CA) (segid 3A4 and resid 346 and name N)	6.21	0.20	0.21
	assign (segid 3A4 and resid 32 and name CA) (segid 3A4 and resid 347 and name CA)	10.68	0.29	0.30
	assign (segid 3A4 and resid 32 and name CA) (segid 3A4 and resid 347 and name CB)	11.70	0.31	0.31
	assign (segid 3A4 and resid 32 and name CA) (segid 3A4 and resid 348 and name CA)	12.02	0.25	0.25
50	assign (segid 3A4 and resid 32 and name CA) (segid 3A4 and resid 349 and name CA)	10.37	0.40	0.39
	assign (segid 3A4 and resid 32 and name CA) (segid 3A4 and resid 349 and name CB)	8.99	0.40	0.40
	assign (segid 3A4 and resid 32 and name CA) (segid 3A4 and resid 34 and name CA)	6.30	0.23	0.22
	assign (segid 3A4 and resid 32 and name CA) (segid 3A4 and resid 34 and name CB)	6.48	0.26	0.25
	assign (segid 3A4 and resid 32 and name CA) (segid 3A4 and resid 34 and name N)	5.28	0.20	0.21
55	assign (segid 3A4 and resid 32 and name CA) (segid 3A4 and resid 350 and name CA)	11.67	0.72	0.71
	assign (segid 3A4 and resid 32 and name CA) (segid 3A4 and resid 350 and name CB)	11.60	0.83	0.82
	assign (segid 3A4 and resid 32 and name CA) (segid 3A4 and resid 351 and name CA)	14.97	0.55	0.55
	assign (segid 3A4 and resid 32 and name CA) (segid 3A4 and resid 352 and name CA)	15.23	0.57	0.57
	assign (segid 3A4 and resid 32 and name CA) (segid 3A4 and resid 352 and name CB)	14.85	0.61	0.62
60	assign (segid 3A4 and resid 32 and name CA) (segid 3A4 and resid 353 and name CA)	14.66	0.70	0.71
	assign (segid 3A4 and resid 32 and name CA) (segid 3A4 and resid 353 and name CB)	14.12	0.83	0.82
	assign (segid 3A4 and resid 32 and name CA) (segid 3A4 and resid 354 and name CA)	17.92	0.68	0.67
	assign (segid 3A4 and resid 32 and name CA) (segid 3A4 and resid 354 and name CB)	18.20	0.63	0.63
	assign (segid 3A4 and resid 32 and name CA) (segid 3A4 and resid 356 and name CA)	17.74	0.78	0.78
65	assign (segid 3A4 and resid 32 and name CA) (segid 3A4 and resid 35 and name CA)	9.51	0.24	0.25
	assign (segid 3A4 and resid 32 and name CA) (segid 3A4 and resid 360 and name CB)	18.64	0.52	0.53
	assign (segid 3A4 and resid 32 and name CA) (segid 3A4 and resid 36 and name CA)	11.99	0.20	0.20
	assign (segid 3A4 and resid 32 and name CA) (segid 3A4 and resid 37 and name CA)	12.99	0.16	0.17
	assign (segid 3A4 and resid 32 and name CA) (segid 3A4 and resid 37 and name CB)	13.56	0.23	0.23
70	assign (segid 3A4 and resid 32 and name CA) (segid 3A4 and resid 381 and name CA)	17.97	0.66	0.66
	assign (segid 3A4 and resid 32 and name CA) (segid 3A4 and resid 382 and name CA)	15.63	0.39	0.39
	assign (segid 3A4 and resid 32 and name CA) (segid 3A4 and resid 382 and name CB)	14.30	0.40	0.41
	assign (segid 3A4 and resid 32 and name CA) (segid 3A4 and resid 383 and name CA)	16.73	0.30	0.30
	assign (segid 3A4 and resid 32 and name CA) (segid 3A4 and resid 384 and name CA)	18.21	0.24	0.25
75	assign (segid 3A4 and resid 32 and name CA) (segid 3A4 and resid 385 and name CA)	15.47	0.40	0.40
	assign (segid 3A4 and resid 32 and name CA) (segid 3A4 and resid 386 and name CA)	16.31	0.35	0.35
	assign (segid 3A4 and resid 32 and name CA) (segid 3A4 and resid 387 and name CA)	17.81	1.05	1.06
	assign (segid 3A4 and resid 32 and name CA) (segid 3A4 and resid 389 and name CA)	18.53	0.67	0.67
	assign (segid 3A4 and resid 32 and name CA) (segid 3A4 and resid 389 and name CB)	17.38	0.69	0.69
80	assign (segid 3A4 and resid 32 and name CA) (segid 3A4 and resid 38 and name CA)	9.88	0.25	0.25
	assign (segid 3A4 and resid 32 and name CA) (segid 3A4 and resid 38 and name CB)	8.76	0.27	0.26
	assign (segid 3A4 and resid 32 and name CA) (segid 3A4 and resid 39 and name CA)	9.43	0.20	0.20

	assign (segid 3A4 and resid 32 and name CA) (segid 3A4 and resid 39 and name CB)	9.42	0.19	0.18
	assign (segid 3A4 and resid 32 and name CA) (segid 3A4 and resid 40 and name CA)	13.16	0.22	0.23
	assign (segid 3A4 and resid 32 and name CA) (segid 3A4 and resid 40 and name CB)	14.28	0.22	0.22
	assign (segid 3A4 and resid 32 and name CA) (segid 3A4 and resid 41 and name CA)	13.14	0.18	0.17
	assign (segid 3A4 and resid 32 and name CA) (segid 3A4 and resid 41 and name CB)	12.81	0.22	0.23
5	assign (segid 3A4 and resid 32 and name CA) (segid 3A4 and resid 429 and name CA)	17.34	1.46	1.46
	assign (segid 3A4 and resid 32 and name CA) (segid 3A4 and resid 42 and name CA)	10.86	0.23	0.23
	assign (segid 3A4 and resid 32 and name CA) (segid 3A4 and resid 42 and name CB)	9.37	0.23	0.23
	assign (segid 3A4 and resid 32 and name CA) (segid 3A4 and resid 430 and name CA)	15.11	2.05	2.05
10	assign (segid 3A4 and resid 32 and name CA) (segid 3A4 and resid 431 and name CA)	15.00	1.25	1.24
	assign (segid 3A4 and resid 32 and name CA) (segid 3A4 and resid 433 and name CA)	18.08	0.78	0.78
	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 317 and name CA)	16.22	0.33	0.32
	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 318 and name CA)	16.93	0.77	0.78
	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 318 and name CB)	18.30	0.73	0.74
	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 319 and name CA)	14.61	0.60	0.61
15	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 319 and name CB)	15.16	0.62	0.62
	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 322 and name CA)	10.17	0.38	0.39
	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 323 and name CA)	11.54	0.19	0.18
	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 323 and name CB)	11.41	0.33	0.33
20	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 324 and name CA)	12.98	0.33	0.32
	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 324 and name CB)	14.07	0.41	0.41
	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 325 and name CA)	14.21	0.29	0.30
	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 325 and name CB)	13.74	0.38	0.38
	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 326 and name CA)	18.01	0.28	0.28
	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 326 and name CB)	18.85	0.28	0.28
25	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 327 and name CA)	18.87	0.41	0.41
	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 328 and name CA)	17.71	0.58	0.58
	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 329 and name CA)	16.22	0.74	0.74
	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 329 and name CB)	15.58	0.83	0.84
	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 330 and name CA)	15.50	0.58	0.58
30	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 330 and name CB)	16.75	0.57	0.57
	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 331 and name CA)	12.96	0.58	0.58
	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 331 and name CB)	11.66	0.57	0.57
	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 332 and name CA)	13.73	0.73	0.73
	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 333 and name CA)	15.52	1.05	1.05
35	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 335 and name CA)	12.83	0.52	0.53
	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 336 and name CA)	14.33	0.48	0.48
	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 336 and name CB)	15.59	0.44	0.45
	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 337 and name CA)	12.66	0.67	0.67
40	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 337 and name CB)	11.87	0.72	0.72
	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 338 and name CA)	15.22	0.57	0.57
	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 338 and name CB)	15.56	0.68	0.68
	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 339 and name CA)	16.85	0.41	0.41
	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 339 and name CB)	18.38	0.41	0.40
45	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 33 and name C)	5.00	0.12	0.11
	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 33 and name CA)	4.71	0.06	0.07
	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 33 and name CB)	5.92	0.08	0.08
	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 33 and name N)	3.46	0.07	0.08
	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 33 and name O)	5.12	0.24	0.24
50	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 340 and name CA)	15.66	0.20	0.21
	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 341 and name CA)	12.05	0.22	0.23
	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 341 and name CB)	11.50	0.32	0.33
	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 342 and name CA)	9.78	0.14	0.13
	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 342 and name O)	7.68	0.17	0.17
	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 343 and name C)	6.78	0.17	0.16
55	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 343 and name CA)	7.08	0.20	0.19
	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 343 and name CB)	7.71	0.25	0.26
	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 344 and name C)	5.33	0.17	0.18
	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 344 and name CA)	5.60	0.14	0.15
60	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 344 and name CB)	5.00	0.27	0.28
	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 344 and name O)	5.57	0.15	0.15
	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 345 and name C)	7.02	0.27	0.28
	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 345 and name CA)	6.77	0.24	0.25
	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 345 and name CB)	8.15	0.28	0.29
65	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 345 and name N)	6.45	0.22	0.21
	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 346 and name CA)	7.04	0.36	0.37
	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 346 and name CB)	6.25	0.45	0.45
	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 346 and name N)	6.44	0.25	0.26
70	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 347 and name CA)	10.76	0.36	0.36
	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 347 and name CB)	11.82	0.39	0.39
	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 348 and name CA)	11.62	0.21	0.21
	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 349 and name CA)	9.94	0.37	0.36
	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 349 and name CB)	8.54	0.38	0.37
	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 34 and name CA)	6.30	0.27	0.28
75	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 34 and name CB)	6.18	0.31	0.32
	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 34 and name N)	5.58	0.23	0.23
	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 350 and name CA)	11.71	0.65	0.65
	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 350 and name CB)	11.81	0.77	0.76
	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 351 and name CA)	14.84	0.49	0.49
80	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 352 and name CA)	14.81	0.52	0.52
	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 352 and name CB)	14.30	0.58	0.58
	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 353 and name CA)	14.46	0.64	0.63

	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 353 and name CB)	14.07	0.76	0.75
	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 354 and name CA)	17.64	0.60	0.59
	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 354 and name CB)	17.83	0.54	0.54
	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 356 and name CB)	17.91	0.70	0.70
	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 35 and name CA)	9.82	0.27	0.27
5	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 360 and name CB)	18.15	0.48	0.48
	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 36 and name CA)	12.47	0.28	0.28
	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 37 and name CA)	13.78	0.23	0.24
	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 37 and name CB)	14.31	0.25	0.26
	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 381 and name CA)	18.17	0.65	0.66
10	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 382 and name CA)	16.02	0.36	0.35
	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 382 and name CB)	14.76	0.36	0.35
	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 383 and name CA)	16.88	0.32	0.32
	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 384 and name CA)	18.60	0.30	0.30
	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 385 and name CA)	16.08	0.45	0.45
15	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 386 and name CA)	17.19	0.39	0.39
	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 389 and name CB)	18.33	0.67	0.68
	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 38 and name CA)	10.90	0.34	0.34
	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 38 and name CB)	9.74	0.36	0.35
	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 39 and name CA)	10.41	0.27	0.27
20	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 39 and name CB)	10.21	0.26	0.26
	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 40 and name CA)	14.20	0.29	0.29
	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 40 and name CB)	15.26	0.29	0.29
	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 41 and name CA)	14.41	0.20	0.21
	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 41 and name CB)	14.09	0.24	0.24
25	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 429 and name CA)	16.40	1.44	1.44
	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 42 and name CA)	12.25	0.25	0.25
	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 42 and name CB)	10.76	0.26	0.25
	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 430 and name CA)	14.31	1.96	1.96
	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 431 and name CA)	14.51	1.08	1.08
30	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 433 and name CA)	17.35	0.78	0.79
	assign (segid 3A4 and resid 32 and name CB) (segid 3A4 and resid 32 and name C)	2.41	0.03	0.03
	assign (segid 3A4 and resid 32 and name N) (segid 3A4 and resid 32 and name CB)	1.46	0.01	0.01
	assign (segid 3A4 and resid 32 and name N) (segid 3A4 and resid 32 and name O)	2.46	0.03	0.03
35	assign (segid 3A4 and resid 32 and name N) (segid 3A4 and resid 32 and name O)	2.84	0.07	0.06
	assign (segid 3A4 and resid 32 and name N) (segid 3A4 and resid 33 and name C)	5.63	0.11	0.11
	assign (segid 3A4 and resid 32 and name N) (segid 3A4 and resid 33 and name CA)	4.67	0.07	0.07
	assign (segid 3A4 and resid 32 and name N) (segid 3A4 and resid 33 and name CB)	5.52	0.05	0.06
	assign (segid 3A4 and resid 32 and name N) (segid 3A4 and resid 33 and name N)	3.41	0.07	0.07
	assign (segid 3A4 and resid 32 and name N) (segid 3A4 and resid 33 and name O)	6.02	0.18	0.17
40	assign (segid 3A4 and resid 32 and name N) (segid 3A4 and resid 342 and name C)	6.61	0.11	0.11
	assign (segid 3A4 and resid 32 and name N) (segid 3A4 and resid 342 and name O)	5.77	0.11	0.11
	assign (segid 3A4 and resid 32 and name N) (segid 3A4 and resid 343 and name C)	5.67	0.16	0.16
	assign (segid 3A4 and resid 32 and name N) (segid 3A4 and resid 343 and name CA)	5.48	0.20	0.20
	assign (segid 3A4 and resid 32 and name N) (segid 3A4 and resid 343 and name CB)	6.00	0.31	0.32
45	assign (segid 3A4 and resid 32 and name N) (segid 3A4 and resid 343 and name N)	6.55	0.14	0.15
	assign (segid 3A4 and resid 32 and name N) (segid 3A4 and resid 343 and name O)	6.84	0.19	0.18
	assign (segid 3A4 and resid 32 and name N) (segid 3A4 and resid 344 and name C)	5.40	0.15	0.14
	assign (segid 3A4 and resid 32 and name N) (segid 3A4 and resid 344 and name CA)	5.43	0.18	0.18
	assign (segid 3A4 and resid 32 and name N) (segid 3A4 and resid 344 and name CB)	5.25	0.32	0.33
50	assign (segid 3A4 and resid 32 and name N) (segid 3A4 and resid 344 and name N)	4.77	0.11	0.15
	assign (segid 3A4 and resid 32 and name N) (segid 3A4 and resid 344 and name O)	4.49	0.17	0.16
	assign (segid 3A4 and resid 32 and name N) (segid 3A4 and resid 345 and name CA)	7.11	0.14	0.15
	assign (segid 3A4 and resid 32 and name N) (segid 3A4 and resid 345 and name N)	6.61	0.16	0.16
	assign (segid 3A4 and resid 32 and name N) (segid 3A4 and resid 346 and name N)	7.55	0.20	0.21
55	assign (segid 3A4 and resid 32 and name N) (segid 3A4 and resid 34 and name CA)	7.46	0.24	0.23
	assign (segid 3A4 and resid 32 and name N) (segid 3A4 and resid 34 and name N)	6.34	0.22	0.22
	assign (segid 3A4 and resid 32 and name N) (segid 3A4 and resid 32 and name CB)	3.00	0.06	0.06
	assign (segid 3A4 and resid 32 and name O) (segid 3A4 and resid 32 and name CB)	3.56	0.13	0.14
	assign (segid 3A4 and resid 32 and name O) (segid 3A4 and resid 33 and name CA)	2.80	0.05	0.05
60	assign (segid 3A4 and resid 32 and name O) (segid 3A4 and resid 33 and name CB)	4.11	0.07	0.07
	assign (segid 3A4 and resid 32 and name O) (segid 3A4 and resid 33 and name N)	2.25	0.02	0.02
	assign (segid 3A4 and resid 32 and name O) (segid 3A4 and resid 33 and name O)	4.36	0.15	0.16
	assign (segid 3A4 and resid 32 and name O) (segid 3A4 and resid 343 and name C)	7.46	0.14	0.14
	assign (segid 3A4 and resid 32 and name O) (segid 3A4 and resid 343 and name CA)	7.41	0.16	0.17
65	assign (segid 3A4 and resid 32 and name O) (segid 3A4 and resid 343 and name CB)	7.48	0.26	0.26
	assign (segid 3A4 and resid 32 and name O) (segid 3A4 and resid 344 and name C)	6.18	0.07	0.07
	assign (segid 3A4 and resid 32 and name O) (segid 3A4 and resid 344 and name CA)	6.85	0.11	0.11
	assign (segid 3A4 and resid 32 and name O) (segid 3A4 and resid 344 and name CB)	6.87	0.30	0.29
	assign (segid 3A4 and resid 32 and name O) (segid 3A4 and resid 344 and name N)	6.50	0.09	0.09
70	assign (segid 3A4 and resid 32 and name O) (segid 3A4 and resid 344 and name O)	5.00	0.08	0.08
	assign (segid 3A4 and resid 32 and name O) (segid 3A4 and resid 345 and name CA)	7.00	0.14	0.15
	assign (segid 3A4 and resid 32 and name O) (segid 3A4 and resid 345 and name N)	7.08	0.11	0.11
	assign (segid 3A4 and resid 32 and name O) (segid 3A4 and resid 346 and name N)	6.95	0.28	0.28
	assign (segid 3A4 and resid 32 and name O) (segid 3A4 and resid 34 and name C)	6.31	0.31	0.31
75	assign (segid 3A4 and resid 32 and name O) (segid 3A4 and resid 34 and name CA)	5.02	0.29	0.30
	assign (segid 3A4 and resid 32 and name O) (segid 3A4 and resid 34 and name CB)	5.08	0.30	0.29
	assign (segid 3A4 and resid 32 and name O) (segid 3A4 and resid 34 and name N)	3.87	0.29	0.28
	assign (segid 3A4 and resid 32 and name O) (segid 3A4 and resid 35 and name N)	7.37	0.30	0.30
80	assign (segid 3A4 and resid 32 and name O) (segid 3A4 and resid 38 and name N)	6.50	0.35	0.34
	assign (segid 3A4 and resid 32 and name O) (segid 3A4 and resid 38 and name CB)	7.18	0.40	0.39
	assign (segid 3A4 and resid 330 and name C) (segid 3A4 and resid 330 and name CB)	2.51	0.02	0.02
	assign (segid 3A4 and resid 330 and name C) (segid 3A4 and resid 330 and name O)	1.23	0.00	0.01

	assign (segid 3A4 and resid 330 and name C) (segid 3A4 and resid 331 and name C)	3.37	0.14	0.14
	assign (segid 3A4 and resid 330 and name C) (segid 3A4 and resid 331 and name CA)	2.45	0.01	0.01
	assign (segid 3A4 and resid 330 and name C) (segid 3A4 and resid 331 and name CB)	3.55	0.07	0.08
	assign (segid 3A4 and resid 330 and name C) (segid 3A4 and resid 331 and name N)	1.33	0.00	0.00
5	assign (segid 3A4 and resid 330 and name C) (segid 3A4 and resid 331 and name O)	3.92	0.19	0.18
	assign (segid 3A4 and resid 330 and name C) (segid 3A4 and resid 332 and name C)	5.33	0.33	0.34
	assign (segid 3A4 and resid 330 and name C) (segid 3A4 and resid 332 and name CA)	5.29	0.22	0.22
	assign (segid 3A4 and resid 330 and name C) (segid 3A4 and resid 332 and name N)	4.07	0.18	0.18
	assign (segid 3A4 and resid 330 and name C) (segid 3A4 and resid 332 and name O)	5.76	0.98	0.98
	assign (segid 3A4 and resid 330 and name C) (segid 3A4 and resid 333 and name C)	5.82	0.33	0.33
10	assign (segid 3A4 and resid 330 and name C) (segid 3A4 and resid 333 and name CA)	5.78	0.44	0.43
	assign (segid 3A4 and resid 330 and name C) (segid 3A4 and resid 333 and name N)	5.20	0.48	0.48
	assign (segid 3A4 and resid 330 and name C) (segid 3A4 and resid 333 and name O)	6.77	0.38	0.37
	assign (segid 3A4 and resid 330 and name C) (segid 3A4 and resid 335 and name C)	4.96	0.37	0.37
	assign (segid 3A4 and resid 330 and name C) (segid 3A4 and resid 335 and name CA)	5.57	0.20	0.20
15	assign (segid 3A4 and resid 330 and name C) (segid 3A4 and resid 335 and name N)	5.11	0.20	0.21
	assign (segid 3A4 and resid 330 and name C) (segid 3A4 and resid 335 and name O)	4.54	1.17	1.17
	assign (segid 3A4 and resid 330 and name C) (segid 3A4 and resid 336 and name C)	5.98	0.27	0.27
	assign (segid 3A4 and resid 330 and name C) (segid 3A4 and resid 336 and name CA)	5.25	0.35	0.36
	assign (segid 3A4 and resid 330 and name C) (segid 3A4 and resid 336 and name CB)	6.30	0.39	0.38
20	assign (segid 3A4 and resid 330 and name C) (segid 3A4 and resid 336 and name N)	5.19	0.46	0.45
	assign (segid 3A4 and resid 330 and name C) (segid 3A4 and resid 336 and name O)	7.12	0.31	0.31
	assign (segid 3A4 and resid 330 and name C) (segid 3A4 and resid 337 and name C)	7.32	0.14	0.15
	assign (segid 3A4 and resid 330 and name C) (segid 3A4 and resid 337 and name CA)	6.55	0.15	0.14
	assign (segid 3A4 and resid 330 and name C) (segid 3A4 and resid 337 and name CB)	6.18	0.28	0.28
25	assign (segid 3A4 and resid 330 and name C) (segid 3A4 and resid 337 and name N)	5.55	0.15	0.15
	assign (segid 3A4 and resid 330 and name C) (segid 3A4 and resid 337 and name O)	6.95	0.14	0.15
	assign (segid 3A4 and resid 330 and name C) (segid 3A4 and resid 330 and name C)	1.52	0.00	0.01
	assign (segid 3A4 and resid 330 and name CA) (segid 3A4 and resid 330 and name CB)	1.53	0.02	0.01
30	assign (segid 3A4 and resid 330 and name CA) (segid 3A4 and resid 330 and name O)	2.41	0.01	0.01
	assign (segid 3A4 and resid 330 and name CA) (segid 3A4 and resid 331 and name C)	4.58	0.08	0.08
	assign (segid 3A4 and resid 330 and name CA) (segid 3A4 and resid 331 and name CA)	3.80	0.01	0.01
	assign (segid 3A4 and resid 330 and name CA) (segid 3A4 and resid 331 and name CB)	4.71	0.07	0.08
	assign (segid 3A4 and resid 330 and name CA) (segid 3A4 and resid 331 and name N)	2.40	0.02	0.02
35	assign (segid 3A4 and resid 330 and name CA) (segid 3A4 and resid 331 and name O)	4.84	0.17	0.18
	assign (segid 3A4 and resid 330 and name CA) (segid 3A4 and resid 332 and name C)	6.21	0.25	0.24
	assign (segid 3A4 and resid 330 and name CA) (segid 3A4 and resid 332 and name CA)	6.45	0.14	0.14
	assign (segid 3A4 and resid 330 and name CA) (segid 3A4 and resid 332 and name N)	5.37	0.11	0.10
	assign (segid 3A4 and resid 330 and name CA) (segid 3A4 and resid 332 and name O)	6.51	0.94	0.95
	assign (segid 3A4 and resid 330 and name CA) (segid 3A4 and resid 333 and name C)	5.97	0.42	0.41
40	assign (segid 3A4 and resid 330 and name CA) (segid 3A4 and resid 333 and name CA)	6.15	0.47	0.47
	assign (segid 3A4 and resid 330 and name CA) (segid 3A4 and resid 333 and name N)	5.91	0.50	0.50
	assign (segid 3A4 and resid 330 and name CA) (segid 3A4 and resid 333 and name O)	6.73	0.53	0.53
	assign (segid 3A4 and resid 330 and name CA) (segid 3A4 and resid 335 and name C)	4.55	0.41	0.41
	assign (segid 3A4 and resid 330 and name CA) (segid 3A4 and resid 335 and name CA)	5.49	0.23	0.24
45	assign (segid 3A4 and resid 330 and name CA) (segid 3A4 and resid 335 and name N)	5.25	0.24	0.25
	assign (segid 3A4 and resid 330 and name CA) (segid 3A4 and resid 335 and name O)	4.15	1.14	1.13
	assign (segid 3A4 and resid 330 and name CA) (segid 3A4 and resid 336 and name C)	5.10	0.18	0.18
	assign (segid 3A4 and resid 330 and name CA) (segid 3A4 and resid 336 and name CA)	4.28	0.24	0.24
50	assign (segid 3A4 and resid 330 and name CA) (segid 3A4 and resid 336 and name CB)	5.13	0.30	0.29
	assign (segid 3A4 and resid 330 and name CA) (segid 3A4 and resid 336 and name N)	4.54	0.29	0.28
	assign (segid 3A4 and resid 330 and name CA) (segid 3A4 and resid 336 and name O)	6.30	0.20	0.20
	assign (segid 3A4 and resid 330 and name CA) (segid 3A4 and resid 337 and name C)	6.45	0.14	0.13
	assign (segid 3A4 and resid 330 and name CA) (segid 3A4 and resid 337 and name CA)	5.86	0.15	0.16
55	assign (segid 3A4 and resid 330 and name CA) (segid 3A4 and resid 337 and name CB)	5.79	0.31	0.32
	assign (segid 3A4 and resid 330 and name CA) (segid 3A4 and resid 337 and name N)	4.73	0.12	0.12
	assign (segid 3A4 and resid 330 and name CA) (segid 3A4 and resid 337 and name O)	5.97	0.15	0.15
	assign (segid 3A4 and resid 330 and name CA) (segid 3A4 and resid 338 and name CA)	8.60	0.11	0.10
	assign (segid 3A4 and resid 330 and name CA) (segid 3A4 and resid 338 and name CB)	9.75	0.14	0.13
60	assign (segid 3A4 and resid 330 and name CA) (segid 3A4 and resid 338 and name N)	7.70	0.12	0.12
	assign (segid 3A4 and resid 330 and name CA) (segid 3A4 and resid 339 and name CA)	10.70	0.22	0.23
	assign (segid 3A4 and resid 330 and name CA) (segid 3A4 and resid 339 and name CB)	11.50	0.26	0.25
	assign (segid 3A4 and resid 330 and name CA) (segid 3A4 and resid 340 and name CA)	13.37	0.27	0.27
	assign (segid 3A4 and resid 330 and name CA) (segid 3A4 and resid 341 and name CA)	12.02	0.28	0.28
	assign (segid 3A4 and resid 330 and name CA) (segid 3A4 and resid 341 and name CB)	10.78	0.29	0.30
65	assign (segid 3A4 and resid 330 and name CA) (segid 3A4 and resid 342 and name CA)	13.79	0.41	0.40
	assign (segid 3A4 and resid 330 and name CA) (segid 3A4 and resid 343 and name CA)	12.67	0.55	0.55
	assign (segid 3A4 and resid 330 and name CA) (segid 3A4 and resid 343 and name CB)	11.50	0.60	0.61
	assign (segid 3A4 and resid 330 and name CA) (segid 3A4 and resid 344 and name CA)	15.55	0.68	0.68
	assign (segid 3A4 and resid 330 and name CA) (segid 3A4 and resid 344 and name CB)	16.55	0.67	0.68
70	assign (segid 3A4 and resid 330 and name CA) (segid 3A4 and resid 345 and name CA)	15.66	0.94	0.94
	assign (segid 3A4 and resid 330 and name CA) (segid 3A4 and resid 345 and name CB)	15.44	0.99	0.99
	assign (segid 3A4 and resid 330 and name CB) (segid 3A4 and resid 331 and name C)	5.25	0.11	0.12
	assign (segid 3A4 and resid 330 and name CB) (segid 3A4 and resid 331 and name CA)	4.77	0.08	0.09
	assign (segid 3A4 and resid 330 and name CB) (segid 3A4 and resid 331 and name CB)	5.92	0.10	0.11
75	assign (segid 3A4 and resid 330 and name CB) (segid 3A4 and resid 331 and name N)	3.49	0.10	0.10
	assign (segid 3A4 and resid 330 and name CB) (segid 3A4 and resid 331 and name O)	5.50	0.27	0.26
	assign (segid 3A4 and resid 330 and name CB) (segid 3A4 and resid 332 and name C)	6.22	0.26	0.26
	assign (segid 3A4 and resid 330 and name CB) (segid 3A4 and resid 332 and name CA)	6.68	0.15	0.15
80	assign (segid 3A4 and resid 330 and name CB) (segid 3A4 and resid 332 and name N)	5.80	0.10	0.10
	assign (segid 3A4 and resid 330 and name CB) (segid 3A4 and resid 332 and name O)	6.45	0.97	0.98
	assign (segid 3A4 and resid 330 and name CB) (segid 3A4 and resid 333 and name C)	5.70	0.59	0.59
	assign (segid 3A4 and resid 330 and name CB) (segid 3A4 and resid 333 and name CA)	5.76	0.63	0.63

	assign (segid 3A4 and resid 330 and name CB)	(segid 3A4 and resid 333 and name N)	5.77	0.62	0.61
	assign (segid 3A4 and resid 330 and name CB)	(segid 3A4 and resid 333 and name O)	6.35	0.76	0.76
	assign (segid 3A4 and resid 330 and name CB)	(segid 3A4 and resid 335 and name C)	4.98	0.44	0.44
	assign (segid 3A4 and resid 330 and name CB)	(segid 3A4 and resid 335 and name CA)	5.82	0.29	0.30
	assign (segid 3A4 and resid 330 and name CB)	(segid 3A4 and resid 335 and name N)	5.38	0.30	0.30
5	assign (segid 3A4 and resid 330 and name CB)	(segid 3A4 and resid 335 and name O)	4.70	1.02	1.03
	assign (segid 3A4 and resid 330 and name CB)	(segid 3A4 and resid 336 and name C)	5.86	0.16	0.16
	assign (segid 3A4 and resid 330 and name CB)	(segid 3A4 and resid 336 and name CA)	4.74	0.18	0.18
	assign (segid 3A4 and resid 330 and name CB)	(segid 3A4 and resid 336 and name CB)	5.20	0.24	0.24
	assign (segid 3A4 and resid 330 and name CB)	(segid 3A4 and resid 336 and name N)	4.94	0.19	0.19
10	assign (segid 3A4 and resid 330 and name CB)	(segid 3A4 and resid 336 and name O)	7.01	0.18	0.17
	assign (segid 3A4 and resid 330 and name CB)	(segid 3A4 and resid 337 and name C)	7.47	0.13	0.13
	assign (segid 3A4 and resid 330 and name CB)	(segid 3A4 and resid 337 and name CA)	7.00	0.18	0.18
	assign (segid 3A4 and resid 330 and name CB)	(segid 3A4 and resid 337 and name CB)	7.14	0.34	0.34
	assign (segid 3A4 and resid 330 and name CB)	(segid 3A4 and resid 337 and name N)	5.73	0.15	0.15
15	assign (segid 3A4 and resid 330 and name CB)	(segid 3A4 and resid 337 and name O)	6.94	0.15	0.14
	assign (segid 3A4 and resid 330 and name CB)	(segid 3A4 and resid 338 and name CA)	9.47	0.07	0.07
	assign (segid 3A4 and resid 330 and name CB)	(segid 3A4 and resid 338 and name CB)	10.54	0.11	0.10
	assign (segid 3A4 and resid 330 and name CB)	(segid 3A4 and resid 339 and name CA)	11.66	0.26	0.26
	assign (segid 3A4 and resid 330 and name CB)	(segid 3A4 and resid 339 and name CB)	12.33	0.31	0.31
20	assign (segid 3A4 and resid 330 and name CB)	(segid 3A4 and resid 340 and name CA)	14.54	0.24	0.23
	assign (segid 3A4 and resid 330 and name CB)	(segid 3A4 and resid 341 and name CA)	13.31	0.26	0.27
	assign (segid 3A4 and resid 330 and name CB)	(segid 3A4 and resid 341 and name CB)	12.06	0.29	0.29
	assign (segid 3A4 and resid 330 and name CB)	(segid 3A4 and resid 342 and name CA)	15.23	0.40	0.39
	assign (segid 3A4 and resid 330 and name CB)	(segid 3A4 and resid 343 and name CA)	14.16	0.55	0.55
25	assign (segid 3A4 and resid 330 and name CB)	(segid 3A4 and resid 343 and name CB)	13.00	0.60	0.61
	assign (segid 3A4 and resid 330 and name CB)	(segid 3A4 and resid 344 and name CA)	17.02	0.69	0.68
	assign (segid 3A4 and resid 330 and name CB)	(segid 3A4 and resid 344 and name CB)	18.00	0.69	0.68
	assign (segid 3A4 and resid 330 and name CB)	(segid 3A4 and resid 345 and name CA)	17.07	0.96	0.95
	assign (segid 3A4 and resid 330 and name CB)	(segid 3A4 and resid 345 and name CB)	16.84	1.01	1.00
30	assign (segid 3A4 and resid 330 and name CB)	(segid 3A4 and resid 330 and name C)	2.41	0.04	0.04
	assign (segid 3A4 and resid 330 and name N)	(segid 3A4 and resid 330 and name CA)	1.45	0.01	0.01
	assign (segid 3A4 and resid 330 and name N)	(segid 3A4 and resid 330 and name CB)	2.44	0.04	0.03
	assign (segid 3A4 and resid 330 and name N)	(segid 3A4 and resid 330 and name O)	2.93	0.18	0.18
	assign (segid 3A4 and resid 330 and name N)	(segid 3A4 and resid 331 and name C)	5.66	0.14	0.13
35	assign (segid 3A4 and resid 330 and name N)	(segid 3A4 and resid 331 and name CA)	4.60	0.11	0.11
	assign (segid 3A4 and resid 330 and name N)	(segid 3A4 and resid 331 and name CB)	5.26	0.15	0.16
	assign (segid 3A4 and resid 330 and name N)	(segid 3A4 and resid 331 and name N)	3.32	0.14	0.14
	assign (segid 3A4 and resid 330 and name N)	(segid 3A4 and resid 331 and name O)	6.00	0.17	0.18
	assign (segid 3A4 and resid 330 and name N)	(segid 3A4 and resid 332 and name C)	7.52	0.27	0.27
40	assign (segid 3A4 and resid 330 and name N)	(segid 3A4 and resid 332 and name CA)	7.64	0.19	0.18
	assign (segid 3A4 and resid 330 and name N)	(segid 3A4 and resid 332 and name N)	6.44	0.16	0.17
	assign (segid 3A4 and resid 330 and name N)	(segid 3A4 and resid 332 and name O)	5.63	0.39	0.40
	assign (segid 3A4 and resid 330 and name N)	(segid 3A4 and resid 335 and name C)	6.71	0.22	0.23
	assign (segid 3A4 and resid 330 and name N)	(segid 3A4 and resid 335 and name N)	6.63	0.25	0.24
45	assign (segid 3A4 and resid 330 and name N)	(segid 3A4 and resid 335 and name O)	5.19	1.08	1.08
	assign (segid 3A4 and resid 330 and name N)	(segid 3A4 and resid 336 and name C)	5.42	0.13	0.12
	assign (segid 3A4 and resid 330 and name N)	(segid 3A4 and resid 336 and name CA)	4.87	0.21	0.21
	assign (segid 3A4 and resid 330 and name N)	(segid 3A4 and resid 336 and name CB)	5.66	0.27	0.26
	assign (segid 3A4 and resid 330 and name N)	(segid 3A4 and resid 336 and name N)	5.46	0.26	0.26
50	assign (segid 3A4 and resid 330 and name N)	(segid 3A4 and resid 336 and name O)	6.64	0.13	0.13
	assign (segid 3A4 and resid 330 and name N)	(segid 3A4 and resid 337 and name C)	5.99	0.09	0.09
	assign (segid 3A4 and resid 330 and name N)	(segid 3A4 and resid 337 and name CA)	5.69	0.10	0.11
	assign (segid 3A4 and resid 330 and name N)	(segid 3A4 and resid 337 and name CB)	5.54	0.28	0.28
	assign (segid 3A4 and resid 330 and name N)	(segid 3A4 and resid 337 and name N)	4.77	0.07	0.07
55	assign (segid 3A4 and resid 330 and name N)	(segid 3A4 and resid 337 and name O)	5.31	0.12	0.11
	assign (segid 3A4 and resid 330 and name N)	(segid 3A4 and resid 338 and name N)	7.26	0.09	0.09
	assign (segid 3A4 and resid 330 and name N)	(segid 3A4 and resid 330 and name CB)	3.00	0.11	0.11
	assign (segid 3A4 and resid 330 and name O)	(segid 3A4 and resid 331 and name C)	3.72	0.30	0.30
60	assign (segid 3A4 and resid 330 and name O)	(segid 3A4 and resid 331 and name CA)	2.82	0.02	0.02
	assign (segid 3A4 and resid 330 and name O)	(segid 3A4 and resid 331 and name CB)	3.98	0.15	0.15
	assign (segid 3A4 and resid 330 and name O)	(segid 3A4 and resid 331 and name N)	2.27	0.02	0.01
	assign (segid 3A4 and resid 330 and name O)	(segid 3A4 and resid 331 and name O)	4.52	0.35	0.34
	assign (segid 3A4 and resid 330 and name O)	(segid 3A4 and resid 332 and name C)	5.52	0.67	0.67
	assign (segid 3A4 and resid 330 and name O)	(segid 3A4 and resid 332 and name CA)	5.32	0.50	0.51
65	assign (segid 3A4 and resid 330 and name O)	(segid 3A4 and resid 332 and name N)	4.08	0.39	0.40
	assign (segid 3A4 and resid 330 and name O)	(segid 3A4 and resid 332 and name O)	5.99	1.28	1.27
	assign (segid 3A4 and resid 330 and name O)	(segid 3A4 and resid 333 and name C)	6.43	0.46	0.45
	assign (segid 3A4 and resid 330 and name O)	(segid 3A4 and resid 333 and name CA)	6.13	0.59	0.59
	assign (segid 3A4 and resid 330 and name O)	(segid 3A4 and resid 333 and name N)	5.43	0.59	0.59
70	assign (segid 3A4 and resid 330 and name O)	(segid 3A4 and resid 335 and name C)	6.05	0.37	0.37
	assign (segid 3A4 and resid 330 and name O)	(segid 3A4 and resid 335 and name CA)	6.56	0.35	0.36
	assign (segid 3A4 and resid 330 and name O)	(segid 3A4 and resid 335 and name N)	5.94	0.39	0.39
	assign (segid 3A4 and resid 330 and name O)	(segid 3A4 and resid 336 and name C)	7.13	0.28	0.28
	assign (segid 3A4 and resid 330 and name O)	(segid 3A4 and resid 336 and name CA)	6.39	0.40	0.40
75	assign (segid 3A4 and resid 330 and name O)	(segid 3A4 and resid 336 and name N)	6.32	0.56	0.57
	assign (segid 3A4 and resid 330 and name O)	(segid 3A4 and resid 337 and name CA)	7.59	0.19	0.19
	assign (segid 3A4 and resid 330 and name O)	(segid 3A4 and resid 337 and name N)	6.65	0.14	0.15
	assign (segid 3A4 and resid 330 and name O)	(segid 3A4 and resid 337 and name CB)	2.52	0.02	0.01
	assign (segid 3A4 and resid 331 and name C)	(segid 3A4 and resid 331 and name O)	1.23	0.01	0.01
80	assign (segid 3A4 and resid 331 and name C)	(segid 3A4 and resid 331 and name O)	2.98	0.07	0.07
	assign (segid 3A4 and resid 331 and name C)	(segid 3A4 and resid 332 and name CA)	2.44	0.02	0.02
	assign (segid 3A4 and resid 331 and name C)	(segid 3A4 and resid 332 and name N)	1.33	0.02	0.01

	assign (segid 3A4 and resid 331 and name C) (segid 3A4 and resid 332 and name O)	3.66	0.40	0.40
	assign (segid 3A4 and resid 331 and name C) (segid 3A4 and resid 333 and name C)	4.71	0.15	0.14
	assign (segid 3A4 and resid 331 and name C) (segid 3A4 and resid 333 and name CA)	4.52	0.21	0.22
	assign (segid 3A4 and resid 331 and name C) (segid 3A4 and resid 333 and name N)	3.38	0.30	0.29
	assign (segid 3A4 and resid 331 and name C) (segid 3A4 and resid 333 and name O)	5.86	0.14	0.14
5	assign (segid 3A4 and resid 331 and name C) (segid 3A4 and resid 335 and name C)	5.07	0.25	0.25
	assign (segid 3A4 and resid 331 and name C) (segid 3A4 and resid 335 and name CA)	4.75	0.12	0.12
	assign (segid 3A4 and resid 331 and name C) (segid 3A4 and resid 335 and name N)	3.97	0.15	0.15
	assign (segid 3A4 and resid 331 and name C) (segid 3A4 and resid 335 and name O)	4.98	0.98	0.97
	assign (segid 3A4 and resid 331 and name C) (segid 3A4 and resid 336 and name C)	7.17	0.32	0.32
10	assign (segid 3A4 and resid 331 and name C) (segid 3A4 and resid 336 and name CA)	6.55	0.39	0.39
	assign (segid 3A4 and resid 331 and name C) (segid 3A4 and resid 336 and name N)	5.75	0.51	0.51
	assign (segid 3A4 and resid 331 and name C) (segid 3A4 and resid 337 and name CB)	7.33	0.12	0.13
	assign (segid 3A4 and resid 331 and name C) (segid 3A4 and resid 337 and name N)	7.00	0.23	0.23
	assign (segid 3A4 and resid 331 and name C) (segid 3A4 and resid 331 and name C)	1.52	0.01	0.01
15	assign (segid 3A4 and resid 331 and name CA) (segid 3A4 and resid 331 and name CB)	1.55	0.01	0.01
	assign (segid 3A4 and resid 331 and name CA) (segid 3A4 and resid 331 and name O)	2.39	0.02	0.01
	assign (segid 3A4 and resid 331 and name CA) (segid 3A4 and resid 332 and name C)	4.39	0.06	0.06
	assign (segid 3A4 and resid 331 and name CA) (segid 3A4 and resid 332 and name CA)	3.81	0.02	0.02
	assign (segid 3A4 and resid 331 and name CA) (segid 3A4 and resid 332 and name N)	2.43	0.02	0.02
20	assign (segid 3A4 and resid 331 and name CA) (segid 3A4 and resid 332 and name O)	5.01	0.51	0.51
	assign (segid 3A4 and resid 331 and name CA) (segid 3A4 and resid 333 and name C)	5.77	0.24	0.24
	assign (segid 3A4 and resid 331 and name CA) (segid 3A4 and resid 333 and name CA)	5.67	0.33	0.34
	assign (segid 3A4 and resid 331 and name CA) (segid 3A4 and resid 333 and name N)	4.63	0.41	0.41
	assign (segid 3A4 and resid 331 and name CA) (segid 3A4 and resid 333 and name O)	6.87	0.22	0.22
25	assign (segid 3A4 and resid 331 and name CA) (segid 3A4 and resid 335 and name C)	5.30	0.37	0.37
	assign (segid 3A4 and resid 331 and name CA) (segid 3A4 and resid 335 and name CA)	5.39	0.19	0.19
	assign (segid 3A4 and resid 331 and name CA) (segid 3A4 and resid 335 and name N)	4.86	0.21	0.21
	assign (segid 3A4 and resid 331 and name CA) (segid 3A4 and resid 335 and name O)	5.02	1.20	1.19
	assign (segid 3A4 and resid 331 and name CA) (segid 3A4 and resid 336 and name C)	6.79	0.38	0.37
30	assign (segid 3A4 and resid 331 and name CA) (segid 3A4 and resid 336 and name CA)	6.32	0.40	0.39
	assign (segid 3A4 and resid 331 and name CA) (segid 3A4 and resid 336 and name CB)	7.61	0.39	0.39
	assign (segid 3A4 and resid 331 and name CA) (segid 3A4 and resid 336 and name N)	5.82	0.50	0.49
	assign (segid 3A4 and resid 331 and name CA) (segid 3A4 and resid 337 and name CA)	7.14	0.17	0.17
	assign (segid 3A4 and resid 331 and name CA) (segid 3A4 and resid 337 and name CB)	6.45	0.14	0.14
35	assign (segid 3A4 and resid 331 and name CA) (segid 3A4 and resid 337 and name N)	6.37	0.24	0.24
	assign (segid 3A4 and resid 331 and name CA) (segid 3A4 and resid 338 and name CA)	10.64	0.21	0.21
	assign (segid 3A4 and resid 331 and name CA) (segid 3A4 and resid 338 and name CB)	11.79	0.24	0.24
	assign (segid 3A4 and resid 331 and name CA) (segid 3A4 and resid 339 and name CA)	12.63	0.22	0.21
	assign (segid 3A4 and resid 331 and name CA) (segid 3A4 and resid 339 and name CB)	13.69	0.22	0.22
40	assign (segid 3A4 and resid 331 and name CA) (segid 3A4 and resid 340 and name CA)	14.50	0.36	0.35
	assign (segid 3A4 and resid 331 and name CA) (segid 3A4 and resid 341 and name CA)	12.46	0.32	0.32
	assign (segid 3A4 and resid 331 and name CA) (segid 3A4 and resid 341 and name CB)	11.24	0.33	0.32
	assign (segid 3A4 and resid 331 and name CA) (segid 3A4 and resid 342 and name CA)	13.21	0.40	0.40
	assign (segid 3A4 and resid 331 and name CA) (segid 3A4 and resid 343 and name CA)	11.12	0.45	0.46
45	assign (segid 3A4 and resid 331 and name CA) (segid 3A4 and resid 343 and name CB)	9.89	0.46	0.47
	assign (segid 3A4 and resid 331 and name CA) (segid 3A4 and resid 344 and name CA)	13.31	0.64	0.63
	assign (segid 3A4 and resid 331 and name CA) (segid 3A4 and resid 344 and name CB)	14.32	0.64	0.65
	assign (segid 3A4 and resid 331 and name CA) (segid 3A4 and resid 345 and name CA)	12.78	0.91	0.90
	assign (segid 3A4 and resid 331 and name CA) (segid 3A4 and resid 345 and name CB)	12.57	0.95	0.94
50	assign (segid 3A4 and resid 331 and name CA) (segid 3A4 and resid 346 and name CA)	15.42	0.98	0.98
	assign (segid 3A4 and resid 331 and name CA) (segid 3A4 and resid 346 and name CB)	15.52	0.95	0.94
	assign (segid 3A4 and resid 331 and name CA) (segid 3A4 and resid 347 and name CA)	17.15	1.05	1.05
	assign (segid 3A4 and resid 331 and name CA) (segid 3A4 and resid 347 and name CB)	18.04	1.05	1.05
	assign (segid 3A4 and resid 331 and name CA) (segid 3A4 and resid 349 and name CA)	17.48	0.99	0.99
55	assign (segid 3A4 and resid 331 and name CA) (segid 3A4 and resid 349 and name CB)	16.42	0.93	0.93
	assign (segid 3A4 and resid 331 and name CA) (segid 3A4 and resid 350 and name CA)	16.20	1.37	1.38
	assign (segid 3A4 and resid 331 and name CA) (segid 3A4 and resid 350 and name CB)	15.67	1.45	1.45
	assign (segid 3A4 and resid 331 and name CA) (segid 3A4 and resid 382 and name CB)	17.43	1.05	1.04
60	assign (segid 3A4 and resid 331 and name CA) (segid 3A4 and resid 386 and name CA)	17.04	0.58	0.58
	assign (segid 3A4 and resid 331 and name CA) (segid 3A4 and resid 387 and name CA)	16.81	0.82	0.82
	assign (segid 3A4 and resid 331 and name CB) (segid 3A4 and resid 332 and name C)	5.47	0.06	0.07
	assign (segid 3A4 and resid 331 and name CB) (segid 3A4 and resid 332 and name CA)	4.76	0.05	0.05
	assign (segid 3A4 and resid 331 and name CB) (segid 3A4 and resid 332 and name N)	3.50	0.04	0.05
65	assign (segid 3A4 and resid 331 and name CB) (segid 3A4 and resid 332 and name O)	6.05	0.41	0.42
	assign (segid 3A4 and resid 331 and name CB) (segid 3A4 and resid 333 and name C)	6.75	0.14	0.14
	assign (segid 3A4 and resid 331 and name CB) (segid 3A4 and resid 333 and name CA)	6.85	0.21	0.21
	assign (segid 3A4 and resid 331 and name CB) (segid 3A4 and resid 333 and name N)	5.81	0.28	0.27
	assign (segid 3A4 and resid 331 and name CB) (segid 3A4 and resid 335 and name C)	5.68	0.45	0.44
	assign (segid 3A4 and resid 331 and name CB) (segid 3A4 and resid 335 and name CA)	5.79	0.35	0.34
70	assign (segid 3A4 and resid 331 and name CB) (segid 3A4 and resid 335 and name N)	5.57	0.30	0.29
	assign (segid 3A4 and resid 331 and name CB) (segid 3A4 and resid 335 and name O)	5.40	1.17	1.18
	assign (segid 3A4 and resid 331 and name CB) (segid 3A4 and resid 336 and name C)	6.76	0.48	0.48
	assign (segid 3A4 and resid 331 and name CB) (segid 3A4 and resid 336 and name CA)	6.62	0.47	0.46
	assign (segid 3A4 and resid 331 and name CB) (segid 3A4 and resid 336 and name CB)	8.04	0.45	0.45
75	assign (segid 3A4 and resid 331 and name CB) (segid 3A4 and resid 336 and name N)	6.17	0.56	0.55
	assign (segid 3A4 and resid 331 and name CB) (segid 3A4 and resid 337 and name CA)	6.69	0.26	0.25
	assign (segid 3A4 and resid 331 and name CB) (segid 3A4 and resid 337 and name CB)	5.77	0.21	0.21
	assign (segid 3A4 and resid 331 and name CB) (segid 3A4 and resid 337 and name N)	6.20	0.33	0.33
	assign (segid 3A4 and resid 331 and name CB) (segid 3A4 and resid 338 and name CA)	10.27	0.30	0.29
80	assign (segid 3A4 and resid 331 and name CB) (segid 3A4 and resid 338 and name CB)	11.41	0.30	0.31
	assign (segid 3A4 and resid 331 and name CB) (segid 3A4 and resid 339 and name CA)	12.12	0.28	0.27
	assign (segid 3A4 and resid 331 and name CB) (segid 3A4 and resid 339 and name CB)	13.28	0.28	0.29

	assign (segid 3A4 and resid 331 and name CB)	(segid 3A4 and resid 340 and name CA)	13.65	0.36	0.36
	assign (segid 3A4 and resid 331 and name CB)	(segid 3A4 and resid 341 and name CA)	11.43	0.34	0.34
	assign (segid 3A4 and resid 331 and name CB)	(segid 3A4 and resid 341 and name CB)	10.25	0.35	0.36
	assign (segid 3A4 and resid 331 and name CB)	(segid 3A4 and resid 342 and name CA)	11.89	0.39	0.40
	assign (segid 3A4 and resid 331 and name CB)	(segid 3A4 and resid 343 and name CA)	9.67	0.45	0.45
5	assign (segid 3A4 and resid 331 and name CB)	(segid 3A4 and resid 343 and name CB)	8.44	0.45	0.46
	assign (segid 3A4 and resid 331 and name CB)	(segid 3A4 and resid 344 and name CA)	11.81	0.66	0.65
	assign (segid 3A4 and resid 331 and name CB)	(segid 3A4 and resid 344 and name CB)	12.84	0.66	0.66
	assign (segid 3A4 and resid 331 and name CB)	(segid 3A4 and resid 345 and name CA)	11.35	0.93	0.93
	assign (segid 3A4 and resid 331 and name CB)	(segid 3A4 and resid 345 and name CB)	11.17	0.98	0.97
10	assign (segid 3A4 and resid 331 and name CB)	(segid 3A4 and resid 346 and name CA)	14.07	0.99	1.00
	assign (segid 3A4 and resid 331 and name CB)	(segid 3A4 and resid 346 and name CB)	14.20	0.96	0.96
	assign (segid 3A4 and resid 331 and name CB)	(segid 3A4 and resid 347 and name CA)	15.91	1.07	1.06
	assign (segid 3A4 and resid 331 and name CB)	(segid 3A4 and resid 347 and name CB)	16.78	1.06	1.06
	assign (segid 3A4 and resid 331 and name CB)	(segid 3A4 and resid 349 and name CA)	16.41	0.97	0.98
15	assign (segid 3A4 and resid 331 and name CB)	(segid 3A4 and resid 349 and name CB)	15.33	0.92	0.92
	assign (segid 3A4 and resid 331 and name CB)	(segid 3A4 and resid 350 and name CA)	15.27	1.37	1.37
	assign (segid 3A4 and resid 331 and name CB)	(segid 3A4 and resid 350 and name CB)	14.71	1.47	1.46
	assign (segid 3A4 and resid 331 and name CB)	(segid 3A4 and resid 382 and name CA)	17.93	1.09	1.09
	assign (segid 3A4 and resid 331 and name CB)	(segid 3A4 and resid 382 and name CB)	16.43	1.07	1.07
20	assign (segid 3A4 and resid 331 and name CB)	(segid 3A4 and resid 385 and name CA)	17.60	0.68	0.68
	assign (segid 3A4 and resid 331 and name CB)	(segid 3A4 and resid 386 and name CA)	16.12	0.63	0.63
	assign (segid 3A4 and resid 331 and name CB)	(segid 3A4 and resid 387 and name CA)	16.01	0.97	0.97
	assign (segid 3A4 and resid 331 and name CB)	(segid 3A4 and resid 389 and name CB)	17.93	0.72	0.72
25	assign (segid 3A4 and resid 331 and name N)	(segid 3A4 and resid 331 and name C)	2.40	0.04	0.04
	assign (segid 3A4 and resid 331 and name N)	(segid 3A4 and resid 331 and name CA)	1.46	0.01	0.02
	assign (segid 3A4 and resid 331 and name N)	(segid 3A4 and resid 331 and name CB)	2.47	0.03	0.04
	assign (segid 3A4 and resid 331 and name N)	(segid 3A4 and resid 331 and name O)	2.84	0.10	0.10
	assign (segid 3A4 and resid 331 and name N)	(segid 3A4 and resid 332 and name C)	4.79	0.10	0.10
30	assign (segid 3A4 and resid 331 and name N)	(segid 3A4 and resid 332 and name CA)	4.64	0.05	0.04
	assign (segid 3A4 and resid 331 and name N)	(segid 3A4 and resid 332 and name N)	3.39	0.04	0.04
	assign (segid 3A4 and resid 331 and name N)	(segid 3A4 and resid 332 and name O)	5.26	0.65	0.66
	assign (segid 3A4 and resid 331 and name N)	(segid 3A4 and resid 333 and name C)	5.41	0.38	0.38
	assign (segid 3A4 and resid 331 and name N)	(segid 3A4 and resid 333 and name CA)	5.50	0.45	0.46
35	assign (segid 3A4 and resid 331 and name N)	(segid 3A4 and resid 333 and name N)	4.78	0.51	0.52
	assign (segid 3A4 and resid 331 and name N)	(segid 3A4 and resid 333 and name O)	6.41	0.39	0.40
	assign (segid 3A4 and resid 331 and name N)	(segid 3A4 and resid 335 and name C)	4.40	0.45	0.45
	assign (segid 3A4 and resid 331 and name N)	(segid 3A4 and resid 335 and name CA)	4.83	0.26	0.26
	assign (segid 3A4 and resid 331 and name N)	(segid 3A4 and resid 335 and name N)	4.45	0.31	0.31
40	assign (segid 3A4 and resid 331 and name N)	(segid 3A4 and resid 335 and name O)	4.02	1.29	1.30
	assign (segid 3A4 and resid 331 and name N)	(segid 3A4 and resid 336 and name C)	5.66	0.32	0.31
	assign (segid 3A4 and resid 331 and name N)	(segid 3A4 and resid 336 and name CA)	5.08	0.35	0.35
	assign (segid 3A4 and resid 331 and name N)	(segid 3A4 and resid 336 and name CB)	6.31	0.34	0.35
	assign (segid 3A4 and resid 331 and name N)	(segid 3A4 and resid 336 and name N)	4.77	0.42	0.41
45	assign (segid 3A4 and resid 331 and name N)	(segid 3A4 and resid 336 and name O)	6.71	0.36	0.36
	assign (segid 3A4 and resid 331 and name N)	(segid 3A4 and resid 337 and name C)	7.19	0.18	0.17
	assign (segid 3A4 and resid 331 and name N)	(segid 3A4 and resid 337 and name CA)	6.19	0.13	0.13
	assign (segid 3A4 and resid 331 and name N)	(segid 3A4 and resid 337 and name CB)	5.72	0.13	0.13
	assign (segid 3A4 and resid 331 and name N)	(segid 3A4 and resid 337 and name N)	5.26	0.20	0.21
50	assign (segid 3A4 and resid 331 and name N)	(segid 3A4 and resid 337 and name O)	7.01	0.22	0.22
	assign (segid 3A4 and resid 331 and name O)	(segid 3A4 and resid 331 and name CB)	2.99	0.09	0.08
	assign (segid 3A4 and resid 331 and name O)	(segid 3A4 and resid 332 and name C)	2.90	0.11	0.10
	assign (segid 3A4 and resid 331 and name O)	(segid 3A4 and resid 332 and name CA)	2.79	0.04	0.03
	assign (segid 3A4 and resid 331 and name O)	(segid 3A4 and resid 332 and name N)	2.25	0.01	0.01
55	assign (segid 3A4 and resid 331 and name O)	(segid 3A4 and resid 332 and name O)	3.43	0.37	0.38
	assign (segid 3A4 and resid 331 and name O)	(segid 3A4 and resid 333 and name C)	3.99	0.11	0.12
	assign (segid 3A4 and resid 331 and name O)	(segid 3A4 and resid 333 and name CA)	4.14	0.14	0.13
	assign (segid 3A4 and resid 331 and name O)	(segid 3A4 and resid 333 and name N)	3.20	0.18	0.19
60	assign (segid 3A4 and resid 331 and name O)	(segid 3A4 and resid 333 and name O)	5.09	0.18	0.18
	assign (segid 3A4 and resid 331 and name O)	(segid 3A4 and resid 335 and name C)	4.24	0.20	0.21
	assign (segid 3A4 and resid 331 and name O)	(segid 3A4 and resid 335 and name CA)	3.73	0.13	0.14
	assign (segid 3A4 and resid 331 and name O)	(segid 3A4 and resid 335 and name N)	3.05	0.13	0.14
	assign (segid 3A4 and resid 331 and name O)	(segid 3A4 and resid 335 and name O)	4.30	0.83	0.83
65	assign (segid 3A4 and resid 331 and name O)	(segid 3A4 and resid 336 and name C)	6.56	0.30	0.31
	assign (segid 3A4 and resid 331 and name O)	(segid 3A4 and resid 336 and name CA)	5.97	0.36	0.37
	assign (segid 3A4 and resid 331 and name O)	(segid 3A4 and resid 336 and name CB)	7.20	0.39	0.38
	assign (segid 3A4 and resid 331 and name O)	(segid 3A4 and resid 336 and name N)	5.00	0.49	0.49
	assign (segid 3A4 and resid 331 and name O)	(segid 3A4 and resid 336 and name O)	7.30	0.33	0.32
	assign (segid 3A4 and resid 331 and name O)	(segid 3A4 and resid 337 and name CB)	7.03	0.28	0.29
	assign (segid 3A4 and resid 331 and name O)	(segid 3A4 and resid 337 and name N)	6.55	0.29	0.28
70	assign (segid 3A4 and resid 332 and name C)	(segid 3A4 and resid 332 and name O)	1.23	0.00	0.01
	assign (segid 3A4 and resid 332 and name C)	(segid 3A4 and resid 333 and name C)	3.23	0.09	0.10
	assign (segid 3A4 and resid 332 and name C)	(segid 3A4 and resid 333 and name CA)	2.44	0.01	0.01
	assign (segid 3A4 and resid 332 and name C)	(segid 3A4 and resid 333 and name N)	1.34	0.01	0.00
75	assign (segid 3A4 and resid 332 and name C)	(segid 3A4 and resid 333 and name O)	4.34	0.14	0.14
	assign (segid 3A4 and resid 332 and name C)	(segid 3A4 and resid 335 and name C)	5.76	0.50	0.51
	assign (segid 3A4 and resid 332 and name C)	(segid 3A4 and resid 335 and name CA)	4.91	0.65	0.65
	assign (segid 3A4 and resid 332 and name C)	(segid 3A4 and resid 335 and name N)	3.58	0.65	0.65
	assign (segid 3A4 and resid 332 and name C)	(segid 3A4 and resid 335 and name O)	5.97	0.59	0.58
80	assign (segid 3A4 and resid 332 and name C)	(segid 3A4 and resid 332 and name C)	1.53	0.01	0.01
	assign (segid 3A4 and resid 332 and name CA)	(segid 3A4 and resid 332 and name O)	2.41	0.02	0.03
	assign (segid 3A4 and resid 332 and name CA)	(segid 3A4 and resid 333 and name C)	4.56	0.08	0.07
	assign (segid 3A4 and resid 332 and name CA)	(segid 3A4 and resid 333 and name CA)	3.81	0.02	0.02

	assign (segid 3A4 and resid 332 and name CA)	(segid 3A4 and resid 333 and name N)	2.44	0.02	0.02
	assign (segid 3A4 and resid 332 and name CA)	(segid 3A4 and resid 333 and name O)	5.68	0.17	0.17
	assign (segid 3A4 and resid 332 and name CA)	(segid 3A4 and resid 335 and name C)	6.51	0.26	0.25
	assign (segid 3A4 and resid 332 and name CA)	(segid 3A4 and resid 335 and name CA)	5.74	0.33	0.33
	assign (segid 3A4 and resid 332 and name CA)	(segid 3A4 and resid 335 and name N)	4.56	0.35	0.35
5	assign (segid 3A4 and resid 332 and name CA)	(segid 3A4 and resid 335 and name O)	6.59	0.69	0.69
	assign (segid 3A4 and resid 332 and name CA)	(segid 3A4 and resid 336 and name CA)	8.33	0.44	0.43
	assign (segid 3A4 and resid 332 and name CA)	(segid 3A4 and resid 336 and name CB)	9.36	0.49	0.49
	assign (segid 3A4 and resid 332 and name CA)	(segid 3A4 and resid 337 and name CA)	10.10	0.20	0.21
	assign (segid 3A4 and resid 332 and name CA)	(segid 3A4 and resid 337 and name CB)	9.67	0.15	0.14
10	assign (segid 3A4 and resid 332 and name CA)	(segid 3A4 and resid 338 and name CA)	13.72	0.20	0.20
	assign (segid 3A4 and resid 332 and name CA)	(segid 3A4 and resid 338 and name CB)	14.70	0.29	0.28
	assign (segid 3A4 and resid 332 and name CA)	(segid 3A4 and resid 339 and name CA)	16.11	0.14	0.14
	assign (segid 3A4 and resid 332 and name CA)	(segid 3A4 and resid 339 and name CB)	17.18	0.18	0.18
	assign (segid 3A4 and resid 332 and name CA)	(segid 3A4 and resid 340 and name CA)	17.95	0.21	0.20
15	assign (segid 3A4 and resid 332 and name CA)	(segid 3A4 and resid 341 and name CA)	15.61	0.15	0.14
	assign (segid 3A4 and resid 332 and name CA)	(segid 3A4 and resid 341 and name CB)	14.30	0.15	0.14
	assign (segid 3A4 and resid 332 and name CA)	(segid 3A4 and resid 342 and name CA)	16.14	0.30	0.30
	assign (segid 3A4 and resid 332 and name CA)	(segid 3A4 and resid 343 and name CA)	13.69	0.41	0.41
	assign (segid 3A4 and resid 332 and name CA)	(segid 3A4 and resid 343 and name CB)	12.58	0.47	0.48
20	assign (segid 3A4 and resid 332 and name CA)	(segid 3A4 and resid 344 and name CA)	15.24	0.61	0.62
	assign (segid 3A4 and resid 332 and name CA)	(segid 3A4 and resid 344 and name CB)	16.09	0.70	0.71
	assign (segid 3A4 and resid 332 and name CA)	(segid 3A4 and resid 345 and name CA)	14.24	0.86	0.86
	assign (segid 3A4 and resid 332 and name CA)	(segid 3A4 and resid 345 and name CB)	14.18	0.87	0.87
	assign (segid 3A4 and resid 332 and name CA)	(segid 3A4 and resid 346 and name CA)	16.18	1.01	1.01
25	assign (segid 3A4 and resid 332 and name CA)	(segid 3A4 and resid 346 and name CB)	16.04	1.01	1.00
	assign (segid 3A4 and resid 332 and name CA)	(segid 3A4 and resid 347 and name CA)	17.77	1.10	1.10
	assign (segid 3A4 and resid 332 and name CA)	(segid 3A4 and resid 349 and name CA)	17.07	1.13	1.14
	assign (segid 3A4 and resid 332 and name CA)	(segid 3A4 and resid 349 and name CB)	16.05	1.06	1.06
	assign (segid 3A4 and resid 332 and name CA)	(segid 3A4 and resid 350 and name CA)	15.75	1.54	1.55
30	assign (segid 3A4 and resid 332 and name CA)	(segid 3A4 and resid 350 and name CB)	15.50	1.55	1.55
	assign (segid 3A4 and resid 332 and name CA)	(segid 3A4 and resid 386 and name CA)	18.52	0.57	0.57
	assign (segid 3A4 and resid 332 and name CA)	(segid 3A4 and resid 387 and name CA)	18.73	0.55	0.56
	assign (segid 3A4 and resid 332 and name N)	(segid 3A4 and resid 332 and name C)	2.46	0.04	0.03
	assign (segid 3A4 and resid 332 and name N)	(segid 3A4 and resid 332 and name CA)	1.46	0.01	0.01
35	assign (segid 3A4 and resid 332 and name N)	(segid 3A4 and resid 332 and name O)	3.27	0.32	0.32
	assign (segid 3A4 and resid 332 and name N)	(segid 3A4 and resid 333 and name C)	4.97	0.14	0.13
	assign (segid 3A4 and resid 332 and name N)	(segid 3A4 and resid 333 and name CA)	4.40	0.21	0.20
	assign (segid 3A4 and resid 332 and name N)	(segid 3A4 and resid 333 and name N)	3.05	0.28	0.28
	assign (segid 3A4 and resid 332 and name N)	(segid 3A4 and resid 333 and name O)	6.14	0.14	0.14
40	assign (segid 3A4 and resid 332 and name N)	(segid 3A4 and resid 335 and name C)	6.11	0.25	0.25
	assign (segid 3A4 and resid 332 and name N)	(segid 3A4 and resid 335 and name CA)	5.65	0.21	0.20
	assign (segid 3A4 and resid 332 and name N)	(segid 3A4 and resid 335 and name N)	4.63	0.25	0.25
	assign (segid 3A4 and resid 332 and name N)	(segid 3A4 and resid 335 and name O)	6.06	0.91	0.90
	assign (segid 3A4 and resid 332 and name N)	(segid 3A4 and resid 336 and name N)	6.82	0.53	0.54
45	assign (segid 3A4 and resid 332 and name O)	(segid 3A4 and resid 333 and name C)	3.35	0.17	0.17
	assign (segid 3A4 and resid 332 and name O)	(segid 3A4 and resid 333 and name CA)	2.77	0.02	0.02
	assign (segid 3A4 and resid 332 and name O)	(segid 3A4 and resid 333 and name N)	2.25	0.02	0.01
	assign (segid 3A4 and resid 332 and name O)	(segid 3A4 and resid 333 and name O)	4.35	0.22	0.21
	assign (segid 3A4 and resid 332 and name O)	(segid 3A4 and resid 335 and name CA)	4.98	0.99	0.98
50	assign (segid 3A4 and resid 332 and name O)	(segid 3A4 and resid 335 and name N)	3.74	0.93	0.92
	assign (segid 3A4 and resid 332 and name O)	(segid 3A4 and resid 335 and name O)	6.23	0.68	0.68
	assign (segid 3A4 and resid 333 and name C)	(segid 3A4 and resid 333 and name O)	1.24	0.01	0.01
	assign (segid 3A4 and resid 333 and name C)	(segid 3A4 and resid 335 and name C)	3.89	0.79	0.79
	assign (segid 3A4 and resid 333 and name C)	(segid 3A4 and resid 335 and name CA)	2.96	0.96	0.97
55	assign (segid 3A4 and resid 333 and name C)	(segid 3A4 and resid 335 and name N)	1.80	0.87	0.87
	assign (segid 3A4 and resid 333 and name C)	(segid 3A4 and resid 335 and name O)	4.31	0.67	0.68
	assign (segid 3A4 and resid 333 and name C)	(segid 3A4 and resid 336 and name CA)	5.86	0.61	0.60
	assign (segid 3A4 and resid 333 and name C)	(segid 3A4 and resid 336 and name CB)	6.37	0.57	0.57
	assign (segid 3A4 and resid 333 and name C)	(segid 3A4 and resid 336 and name N)	4.67	0.74	0.75
60	assign (segid 3A4 and resid 333 and name C)	(segid 3A4 and resid 333 and name C)	1.52	0.01	0.01
	assign (segid 3A4 and resid 333 and name CA)	(segid 3A4 and resid 333 and name O)	2.39	0.02	0.02
	assign (segid 3A4 and resid 333 and name CA)	(segid 3A4 and resid 335 and name C)	5.06	0.60	0.61
	assign (segid 3A4 and resid 333 and name CA)	(segid 3A4 and resid 335 and name CA)	4.26	0.80	0.79
	assign (segid 3A4 and resid 333 and name CA)	(segid 3A4 and resid 335 and name N)	2.88	0.79	0.79
65	assign (segid 3A4 and resid 333 and name CA)	(segid 3A4 and resid 335 and name O)	5.31	0.56	0.56
	assign (segid 3A4 and resid 333 and name CA)	(segid 3A4 and resid 336 and name CA)	6.92	0.41	0.42
	assign (segid 3A4 and resid 333 and name CA)	(segid 3A4 and resid 336 and name CB)	7.45	0.44	0.44
	assign (segid 3A4 and resid 333 and name CA)	(segid 3A4 and resid 336 and name N)	5.85	0.59	0.58
	assign (segid 3A4 and resid 333 and name CA)	(segid 3A4 and resid 337 and name CA)	9.79	0.39	0.39
70	assign (segid 3A4 and resid 333 and name CA)	(segid 3A4 and resid 337 and name CB)	9.89	0.39	0.40
	assign (segid 3A4 and resid 333 and name CA)	(segid 3A4 and resid 338 and name CA)	13.06	0.39	0.39
	assign (segid 3A4 and resid 333 and name CA)	(segid 3A4 and resid 338 and name CB)	13.83	0.47	0.46
	assign (segid 3A4 and resid 333 and name CA)	(segid 3A4 and resid 339 and name CA)	15.95	0.38	0.38
	assign (segid 3A4 and resid 333 and name CA)	(segid 3A4 and resid 339 and name CB)	16.89	0.42	0.42
75	assign (segid 3A4 and resid 333 and name CA)	(segid 3A4 and resid 340 and name CA)	18.21	0.26	0.25
	assign (segid 3A4 and resid 333 and name CA)	(segid 3A4 and resid 341 and name CA)	16.00	0.31	0.32
	assign (segid 3A4 and resid 333 and name CA)	(segid 3A4 and resid 341 and name CB)	14.57	0.32	0.33
	assign (segid 3A4 and resid 333 and name CA)	(segid 3A4 and resid 342 and name CA)	17.26	0.44	0.44
	assign (segid 3A4 and resid 333 and name CA)	(segid 3A4 and resid 343 and name CA)	15.44	0.52	0.52
80	assign (segid 3A4 and resid 333 and name CA)	(segid 3A4 and resid 343 and name CB)	14.47	0.62	0.61
	assign (segid 3A4 and resid 333 and name CA)	(segid 3A4 and resid 344 and name CA)	17.46	0.67	0.68
	assign (segid 3A4 and resid 333 and name CA)	(segid 3A4 and resid 344 and name CB)	18.19	0.76	0.76

	assign (segid 3A4 and resid 333 and name CA)	(segid 3A4 and resid 345 and name CA)	17.08	0.87	0.87
	assign (segid 3A4 and resid 333 and name CA)	(segid 3A4 and resid 345 and name CB)	17.15	0.89	0.89
	assign (segid 3A4 and resid 333 and name N)	(segid 3A4 and resid 333 and name C)	2.47	0.05	0.04
	assign (segid 3A4 and resid 333 and name N)	(segid 3A4 and resid 333 and name CA)	1.45	0.01	0.01
	assign (segid 3A4 and resid 333 and name N)	(segid 3A4 and resid 333 and name O)	3.54	0.13	0.13
5	assign (segid 3A4 and resid 333 and name N)	(segid 3A4 and resid 335 and name C)	5.34	0.41	0.41
	assign (segid 3A4 and resid 333 and name N)	(segid 3A4 and resid 335 and name CA)	4.55	0.55	0.54
	assign (segid 3A4 and resid 333 and name N)	(segid 3A4 and resid 335 and name N)	3.15	0.58	0.58
	assign (segid 3A4 and resid 333 and name N)	(segid 3A4 and resid 335 and name O)	5.48	0.64	0.63
10	assign (segid 3A4 and resid 333 and name N)	(segid 3A4 and resid 336 and name CA)	7.24	0.26	0.26
	assign (segid 3A4 and resid 333 and name N)	(segid 3A4 and resid 336 and name N)	6.18	0.43	0.43
	assign (segid 3A4 and resid 333 and name O)	(segid 3A4 and resid 335 and name C)	4.22	0.92	0.93
	assign (segid 3A4 and resid 333 and name O)	(segid 3A4 and resid 335 and name CA)	3.35	1.07	1.06
	assign (segid 3A4 and resid 333 and name O)	(segid 3A4 and resid 335 and name N)	2.68	0.80	0.80
15	assign (segid 3A4 and resid 333 and name O)	(segid 3A4 and resid 335 and name O)	4.73	0.80	0.80
	assign (segid 3A4 and resid 335 and name C)	(segid 3A4 and resid 336 and name CA)	6.03	0.78	0.79
	assign (segid 3A4 and resid 335 and name C)	(segid 3A4 and resid 336 and name N)	4.87	0.90	0.90
	assign (segid 3A4 and resid 335 and name C)	(segid 3A4 and resid 336 and name O)	1.24	0.01	0.00
	assign (segid 3A4 and resid 335 and name C)	(segid 3A4 and resid 336 and name C)	3.25	0.11	0.10
20	assign (segid 3A4 and resid 335 and name C)	(segid 3A4 and resid 336 and name CA)	2.44	0.02	0.01
	assign (segid 3A4 and resid 335 and name C)	(segid 3A4 and resid 336 and name CB)	3.37	0.26	0.26
	assign (segid 3A4 and resid 335 and name C)	(segid 3A4 and resid 336 and name N)	1.33	0.01	0.01
	assign (segid 3A4 and resid 335 and name C)	(segid 3A4 and resid 336 and name O)	3.75	0.25	0.25
	assign (segid 3A4 and resid 335 and name C)	(segid 3A4 and resid 337 and name C)	6.31	0.24	0.23
25	assign (segid 3A4 and resid 335 and name C)	(segid 3A4 and resid 337 and name CA)	5.16	0.24	0.24
	assign (segid 3A4 and resid 335 and name C)	(segid 3A4 and resid 337 and name CB)	5.65	0.37	0.37
	assign (segid 3A4 and resid 335 and name C)	(segid 3A4 and resid 337 and name N)	3.96	0.26	0.25
	assign (segid 3A4 and resid 335 and name C)	(segid 3A4 and resid 337 and name O)	6.63	0.28	0.29
	assign (segid 3A4 and resid 335 and name C)	(segid 3A4 and resid 338 and name N)	7.16	0.25	0.24
30	assign (segid 3A4 and resid 335 and name CA)	(segid 3A4 and resid 335 and name C)	1.53	0.01	0.01
	assign (segid 3A4 and resid 335 and name CA)	(segid 3A4 and resid 335 and name O)	2.39	0.01	0.01
	assign (segid 3A4 and resid 335 and name CA)	(segid 3A4 and resid 336 and name C)	4.57	0.08	0.08
	assign (segid 3A4 and resid 335 and name CA)	(segid 3A4 and resid 336 and name CA)	3.82	0.02	0.02
	assign (segid 3A4 and resid 335 and name CA)	(segid 3A4 and resid 336 and name CB)	4.65	0.16	0.17
35	assign (segid 3A4 and resid 335 and name CA)	(segid 3A4 and resid 336 and name N)	2.45	0.02	0.02
	assign (segid 3A4 and resid 335 and name CA)	(segid 3A4 and resid 336 and name O)	4.89	0.18	0.18
	assign (segid 3A4 and resid 335 and name CA)	(segid 3A4 and resid 337 and name CA)	6.37	0.21	0.22
	assign (segid 3A4 and resid 335 and name CA)	(segid 3A4 and resid 337 and name CB)	6.72	0.28	0.27
	assign (segid 3A4 and resid 335 and name CA)	(segid 3A4 and resid 337 and name N)	5.28	0.21	0.20
40	assign (segid 3A4 and resid 335 and name CA)	(segid 3A4 and resid 338 and name CA)	9.75	0.29	0.28
	assign (segid 3A4 and resid 335 and name CA)	(segid 3A4 and resid 338 and name CB)	10.33	0.29	0.28
	assign (segid 3A4 and resid 335 and name CA)	(segid 3A4 and resid 339 and name CA)	12.98	0.31	0.31
	assign (segid 3A4 and resid 335 and name CA)	(segid 3A4 and resid 339 and name CB)	14.07	0.35	0.36
	assign (segid 3A4 and resid 335 and name CA)	(segid 3A4 and resid 340 and name CA)	14.88	0.26	0.25
45	assign (segid 3A4 and resid 335 and name CA)	(segid 3A4 and resid 341 and name CA)	12.36	0.38	0.38
	assign (segid 3A4 and resid 335 and name CA)	(segid 3A4 and resid 341 and name CB)	10.88	0.37	0.37
	assign (segid 3A4 and resid 335 and name CA)	(segid 3A4 and resid 342 and name CA)	13.79	0.51	0.52
	assign (segid 3A4 and resid 335 and name CA)	(segid 3A4 and resid 343 and name CA)	12.42	0.55	0.55
	assign (segid 3A4 and resid 335 and name CA)	(segid 3A4 and resid 343 and name CB)	11.68	0.64	0.64
50	assign (segid 3A4 and resid 335 and name CA)	(segid 3A4 and resid 344 and name CA)	14.79	0.57	0.58
	assign (segid 3A4 and resid 335 and name CA)	(segid 3A4 and resid 344 and name CB)	15.38	0.64	0.64
	assign (segid 3A4 and resid 335 and name CA)	(segid 3A4 and resid 345 and name CA)	15.22	0.70	0.70
	assign (segid 3A4 and resid 335 and name CA)	(segid 3A4 and resid 345 and name CB)	15.50	0.73	0.74
	assign (segid 3A4 and resid 335 and name CA)	(segid 3A4 and resid 346 and name CA)	17.42	0.74	0.74
55	assign (segid 3A4 and resid 335 and name CA)	(segid 3A4 and resid 346 and name CB)	17.11	0.74	0.73
	assign (segid 3A4 and resid 335 and name CA)	(segid 3A4 and resid 349 and name CB)	17.95	0.83	0.82
	assign (segid 3A4 and resid 335 and name N)	(segid 3A4 and resid 335 and name C)	2.50	0.08	0.08
	assign (segid 3A4 and resid 335 and name N)	(segid 3A4 and resid 335 and name CA)	1.46	0.00	0.00
	assign (segid 3A4 and resid 335 and name N)	(segid 3A4 and resid 335 and name O)	3.05	0.29	0.29
60	assign (segid 3A4 and resid 335 and name N)	(segid 3A4 and resid 336 and name C)	5.65	0.09	0.10
	assign (segid 3A4 and resid 335 and name N)	(segid 3A4 and resid 336 and name CA)	4.69	0.07	0.08
	assign (segid 3A4 and resid 335 and name N)	(segid 3A4 and resid 336 and name CB)	5.46	0.22	0.22
	assign (segid 3A4 and resid 335 and name N)	(segid 3A4 and resid 336 and name N)	3.40	0.13	0.13
	assign (segid 3A4 and resid 335 and name N)	(segid 3A4 and resid 336 and name O)	6.16	0.19	0.19
65	assign (segid 3A4 and resid 335 and name N)	(segid 3A4 and resid 337 and name CA)	7.39	0.21	0.21
	assign (segid 3A4 and resid 335 and name N)	(segid 3A4 and resid 337 and name N)	6.23	0.19	0.18
	assign (segid 3A4 and resid 335 and name O)	(segid 3A4 and resid 336 and name C)	3.41	0.20	0.20
	assign (segid 3A4 and resid 335 and name O)	(segid 3A4 and resid 336 and name CA)	2.77	0.03	0.03
	assign (segid 3A4 and resid 335 and name O)	(segid 3A4 and resid 336 and name CB)	3.61	0.54	0.54
70	assign (segid 3A4 and resid 335 and name O)	(segid 3A4 and resid 336 and name N)	2.25	0.01	0.01
	assign (segid 3A4 and resid 335 and name O)	(segid 3A4 and resid 336 and name O)	3.95	0.53	0.53
	assign (segid 3A4 and resid 335 and name O)	(segid 3A4 and resid 337 and name C)	6.14	0.36	0.36
	assign (segid 3A4 and resid 335 and name O)	(segid 3A4 and resid 337 and name CA)	5.04	0.42	0.42
	assign (segid 3A4 and resid 335 and name O)	(segid 3A4 and resid 337 and name CB)	5.41	0.73	0.74
75	assign (segid 3A4 and resid 335 and name O)	(segid 3A4 and resid 337 and name N)	3.90	0.44	0.44
	assign (segid 3A4 and resid 335 and name O)	(segid 3A4 and resid 337 and name O)	6.41	0.49	0.49
	assign (segid 3A4 and resid 335 and name O)	(segid 3A4 and resid 338 and name N)	7.01	0.28	0.29
	assign (segid 3A4 and resid 336 and name C)	(segid 3A4 and resid 336 and name CB)	2.52	0.04	0.03
	assign (segid 3A4 and resid 336 and name C)	(segid 3A4 and resid 336 and name O)	1.24	0.01	0.00
80	assign (segid 3A4 and resid 336 and name C)	(segid 3A4 and resid 337 and name C)	3.29	0.13	0.12
	assign (segid 3A4 and resid 336 and name C)	(segid 3A4 and resid 337 and name CA)	2.44	0.01	0.02
	assign (segid 3A4 and resid 336 and name C)	(segid 3A4 and resid 337 and name CB)	3.59	0.09	0.09
	assign (segid 3A4 and resid 336 and name C)	(segid 3A4 and resid 337 and name N)	1.33	0.01	0.00

	assign (segid 3A4 and resid 336 and name C)	(segid 3A4 and resid 337 and name O)	3.77	0.12	0.12
	assign (segid 3A4 and resid 336 and name C)	(segid 3A4 and resid 338 and name C)	6.38	0.28	0.27
	assign (segid 3A4 and resid 336 and name C)	(segid 3A4 and resid 338 and name CA)	5.24	0.26	0.26
	assign (segid 3A4 and resid 336 and name C)	(segid 3A4 and resid 338 and name CB)	5.89	0.23	0.24
	assign (segid 3A4 and resid 336 and name C)	(segid 3A4 and resid 338 and name N)	4.02	0.22	0.23
5	assign (segid 3A4 and resid 336 and name C)	(segid 3A4 and resid 338 and name O)	6.62	0.27	0.28
	assign (segid 3A4 and resid 336 and name C)	(segid 3A4 and resid 339 and name N)	7.35	0.29	0.29
	assign (segid 3A4 and resid 336 and name C)	(segid 3A4 and resid 341 and name CB)	7.39	0.22	0.21
	assign (segid 3A4 and resid 336 and name C)	(segid 3A4 and resid 341 and name CG)	6.84	0.27	0.27
	assign (segid 3A4 and resid 336 and name C)	(segid 3A4 and resid 336 and name C)	1.52	0.01	0.02
10	assign (segid 3A4 and resid 336 and name CA)	(segid 3A4 and resid 336 and name CB)	1.52	0.01	0.01
	assign (segid 3A4 and resid 336 and name CA)	(segid 3A4 and resid 336 and name O)	2.42	0.02	0.01
	assign (segid 3A4 and resid 336 and name CA)	(segid 3A4 and resid 337 and name C)	4.52	0.10	0.10
	assign (segid 3A4 and resid 336 and name CA)	(segid 3A4 and resid 337 and name CA)	3.79	0.03	0.02
	assign (segid 3A4 and resid 336 and name CA)	(segid 3A4 and resid 337 and name CB)	4.73	0.06	0.05
15	assign (segid 3A4 and resid 336 and name CA)	(segid 3A4 and resid 337 and name N)	2.40	0.04	0.03
	assign (segid 3A4 and resid 336 and name CA)	(segid 3A4 and resid 337 and name O)	4.69	0.12	0.12
	assign (segid 3A4 and resid 336 and name CA)	(segid 3A4 and resid 338 and name CA)	6.44	0.24	0.24
	assign (segid 3A4 and resid 336 and name CA)	(segid 3A4 and resid 338 and name CB)	7.11	0.22	0.22
	assign (segid 3A4 and resid 336 and name CA)	(segid 3A4 and resid 338 and name N)	5.36	0.20	0.20
20	assign (segid 3A4 and resid 336 and name CA)	(segid 3A4 and resid 339 and name CA)	9.71	0.33	0.33
	assign (segid 3A4 and resid 336 and name CA)	(segid 3A4 and resid 339 and name CB)	10.65	0.40	0.39
	assign (segid 3A4 and resid 336 and name CA)	(segid 3A4 and resid 340 and name CA)	12.13	0.11	0.10
	assign (segid 3A4 and resid 336 and name CA)	(segid 3A4 and resid 341 and name CA)	10.29	0.18	0.19
	assign (segid 3A4 and resid 336 and name CA)	(segid 3A4 and resid 341 and name CB)	8.87	0.20	0.20
25	assign (segid 3A4 and resid 336 and name CA)	(segid 3A4 and resid 342 and name CA)	12.58	0.31	0.30
	assign (segid 3A4 and resid 336 and name CA)	(segid 3A4 and resid 343 and name CA)	12.10	0.32	0.32
	assign (segid 3A4 and resid 336 and name CA)	(segid 3A4 and resid 343 and name CB)	11.34	0.42	0.42
	assign (segid 3A4 and resid 336 and name CA)	(segid 3A4 and resid 344 and name CA)	15.19	0.43	0.42
	assign (segid 3A4 and resid 336 and name CA)	(segid 3A4 and resid 344 and name CB)	15.88	0.40	0.40
30	assign (segid 3A4 and resid 336 and name CA)	(segid 3A4 and resid 345 and name CA)	16.16	0.71	0.71
	assign (segid 3A4 and resid 336 and name CA)	(segid 3A4 and resid 345 and name CB)	16.29	0.81	0.81
	assign (segid 3A4 and resid 336 and name CA)	(segid 3A4 and resid 346 and name CA)	18.89	0.67	0.68
	assign (segid 3A4 and resid 336 and name CA)	(segid 3A4 and resid 346 and name CB)	18.79	0.63	0.62
	assign (segid 3A4 and resid 336 and name CA)	(segid 3A4 and resid 337 and name C)	5.16	0.13	0.12
35	assign (segid 3A4 and resid 336 and name CB)	(segid 3A4 and resid 337 and name CA)	4.78	0.03	0.03
	assign (segid 3A4 and resid 336 and name CB)	(segid 3A4 and resid 337 and name CB)	5.94	0.06	0.05
	assign (segid 3A4 and resid 336 and name CB)	(segid 3A4 and resid 337 and name N)	3.51	0.05	0.04
	assign (segid 3A4 and resid 336 and name CB)	(segid 3A4 and resid 337 and name O)	5.24	0.20	0.20
	assign (segid 3A4 and resid 336 and name CB)	(segid 3A4 and resid 338 and name CA)	6.65	0.31	0.30
40	assign (segid 3A4 and resid 336 and name CB)	(segid 3A4 and resid 338 and name CB)	7.12	0.29	0.30
	assign (segid 3A4 and resid 336 and name CB)	(segid 3A4 and resid 338 and name N)	5.81	0.24	0.23
	assign (segid 3A4 and resid 336 and name CB)	(segid 3A4 and resid 339 and name CA)	10.02	0.45	0.45
	assign (segid 3A4 and resid 336 and name CB)	(segid 3A4 and resid 339 and name CB)	10.80	0.53	0.53
	assign (segid 3A4 and resid 336 and name CB)	(segid 3A4 and resid 340 and name CA)	12.65	0.20	0.19
45	assign (segid 3A4 and resid 336 and name CB)	(segid 3A4 and resid 341 and name CA)	11.05	0.17	0.18
	assign (segid 3A4 and resid 336 and name CB)	(segid 3A4 and resid 341 and name CB)	9.67	0.20	0.20
	assign (segid 3A4 and resid 336 and name CB)	(segid 3A4 and resid 342 and name CA)	13.61	0.30	0.30
	assign (segid 3A4 and resid 336 and name CB)	(segid 3A4 and resid 343 and name CB)	13.41	0.34	0.33
	assign (segid 3A4 and resid 336 and name CB)	(segid 3A4 and resid 343 and name CB)	12.70	0.44	0.44
50	assign (segid 3A4 and resid 336 and name CB)	(segid 3A4 and resid 344 and name CA)	16.56	0.42	0.42
	assign (segid 3A4 and resid 336 and name CB)	(segid 3A4 and resid 344 and name CB)	17.21	0.39	0.39
	assign (segid 3A4 and resid 336 and name CB)	(segid 3A4 and resid 345 and name CA)	17.63	0.70	0.70
	assign (segid 3A4 and resid 336 and name CB)	(segid 3A4 and resid 345 and name CB)	17.78	0.82	0.81
	assign (segid 3A4 and resid 336 and name CB)	(segid 3A4 and resid 336 and name C)	2.16	0.04	0.05
55	assign (segid 3A4 and resid 336 and name N)	(segid 3A4 and resid 336 and name CA)	1.46	0.01	0.01
	assign (segid 3A4 and resid 336 and name N)	(segid 3A4 and resid 336 and name CB)	2.45	0.07	0.08
	assign (segid 3A4 and resid 336 and name N)	(segid 3A4 and resid 336 and name O)	3.04	0.09	0.08
	assign (segid 3A4 and resid 336 and name N)	(segid 3A4 and resid 337 and name C)	5.65	0.14	0.14
	assign (segid 3A4 and resid 336 and name N)	(segid 3A4 and resid 337 and name CA)	4.64	0.09	0.09
60	assign (segid 3A4 and resid 336 and name N)	(segid 3A4 and resid 337 and name CB)	5.35	0.08	0.08
	assign (segid 3A4 and resid 336 and name N)	(segid 3A4 and resid 337 and name N)	3.35	0.10	0.10
	assign (segid 3A4 and resid 336 and name N)	(segid 3A4 and resid 337 and name O)	5.95	0.12	0.11
	assign (segid 3A4 and resid 336 and name N)	(segid 3A4 and resid 338 and name N)	6.48	0.25	0.24
	assign (segid 3A4 and resid 336 and name N)	(segid 3A4 and resid 336 and name CB)	2.99	0.10	0.10
65	assign (segid 3A4 and resid 336 and name O)	(segid 3A4 and resid 337 and name C)	3.59	0.19	0.19
	assign (segid 3A4 and resid 336 and name O)	(segid 3A4 and resid 337 and name CA)	2.82	0.04	0.03
	assign (segid 3A4 and resid 336 and name O)	(segid 3A4 and resid 337 and name CB)	4.08	0.16	0.16
	assign (segid 3A4 and resid 336 and name O)	(segid 3A4 and resid 337 and name N)	2.27	0.02	0.02
	assign (segid 3A4 and resid 336 and name O)	(segid 3A4 and resid 337 and name O)	4.34	0.17	0.18
70	assign (segid 3A4 and resid 336 and name O)	(segid 3A4 and resid 338 and name C)	6.39	0.37	0.36
	assign (segid 3A4 and resid 336 and name O)	(segid 3A4 and resid 338 and name CA)	5.16	0.40	0.39
	assign (segid 3A4 and resid 336 and name O)	(segid 3A4 and resid 338 and name CB)	5.53	0.39	0.39
	assign (segid 3A4 and resid 336 and name O)	(segid 3A4 and resid 338 and name N)	3.94	0.34	0.34
	assign (segid 3A4 and resid 336 and name O)	(segid 3A4 and resid 338 and name O)	6.61	0.32	0.31
75	assign (segid 3A4 and resid 336 and name O)	(segid 3A4 and resid 341 and name CB)	7.06	0.30	0.31
	assign (segid 3A4 and resid 336 and name O)	(segid 3A4 and resid 341 and name CG)	6.37	0.33	0.33
	assign (segid 3A4 and resid 337 and name C)	(segid 3A4 and resid 337 and name CB)	2.53	0.03	0.04
	assign (segid 3A4 and resid 337 and name C)	(segid 3A4 and resid 337 and name O)	1.23	0.00	0.00
	assign (segid 3A4 and resid 337 and name C)	(segid 3A4 and resid 338 and name C)	3.73	0.12	0.12
80	assign (segid 3A4 and resid 337 and name C)	(segid 3A4 and resid 338 and name CA)	2.45	0.03	0.02
	assign (segid 3A4 and resid 337 and name C)	(segid 3A4 and resid 338 and name CB)	3.62	0.04	0.03
	assign (segid 3A4 and resid 337 and name C)	(segid 3A4 and resid 338 and name N)	1.33	0.02	0.01

	assign (segid 3A4 and resid 337 and name C) (segid 3A4 and resid 338 and name O)	3.48	0.22	0.22
	assign (segid 3A4 and resid 337 and name C) (segid 3A4 and resid 339 and name C)	6.05	0.10	0.11
	assign (segid 3A4 and resid 337 and name C) (segid 3A4 and resid 339 and name CA)	5.41	0.13	0.13
	assign (segid 3A4 and resid 337 and name C) (segid 3A4 and resid 339 and name CB)	6.57	0.13	0.13
5	assign (segid 3A4 and resid 337 and name C) (segid 3A4 and resid 339 and name N)	4.24	0.09	0.08
	assign (segid 3A4 and resid 337 and name C) (segid 3A4 and resid 339 and name O)	6.26	0.15	0.15
	assign (segid 3A4 and resid 337 and name C) (segid 3A4 and resid 340 and name C)	7.38	0.06	0.07
	assign (segid 3A4 and resid 337 and name C) (segid 3A4 and resid 340 and name CA)	7.67	0.05	0.06
	assign (segid 3A4 and resid 337 and name C) (segid 3A4 and resid 340 and name N)	6.69	0.05	0.05
	assign (segid 3A4 and resid 337 and name C) (segid 3A4 and resid 341 and name C)	7.16	0.21	0.20
10	assign (segid 3A4 and resid 337 and name C) (segid 3A4 and resid 341 and name CA)	6.31	0.09	0.10
	assign (segid 3A4 and resid 337 and name C) (segid 3A4 and resid 341 and name CB)	5.10	0.09	0.10
	assign (segid 3A4 and resid 337 and name C) (segid 3A4 and resid 341 and name CG)	4.65	0.24	0.24
	assign (segid 3A4 and resid 337 and name C) (segid 3A4 and resid 341 and name N)	6.22	0.06	0.06
	assign (segid 3A4 and resid 337 and name C) (segid 3A4 and resid 341 and name O)	7.15	0.30	0.29
15	assign (segid 3A4 and resid 337 and name C) (segid 3A4 and resid 337 and name C)	1.53	0.01	0.00
	assign (segid 3A4 and resid 337 and name CA) (segid 3A4 and resid 337 and name CB)	1.54	0.03	0.02
	assign (segid 3A4 and resid 337 and name CA) (segid 3A4 and resid 337 and name O)	2.40	0.01	0.01
	assign (segid 3A4 and resid 337 and name CA) (segid 3A4 and resid 338 and name C)	4.57	0.08	0.07
	assign (segid 3A4 and resid 337 and name CA) (segid 3A4 and resid 338 and name CB)	3.83	0.02	0.01
20	assign (segid 3A4 and resid 337 and name CA) (segid 3A4 and resid 338 and name N)	4.79	0.05	0.05
	assign (segid 3A4 and resid 337 and name CA) (segid 3A4 and resid 338 and name O)	2.44	0.02	0.03
	assign (segid 3A4 and resid 337 and name CA) (segid 3A4 and resid 338 and name O)	4.53	0.17	0.17
	assign (segid 3A4 and resid 337 and name CA) (segid 3A4 and resid 339 and name C)	7.27	0.06	0.06
	assign (segid 3A4 and resid 337 and name CA) (segid 3A4 and resid 339 and name CA)	6.75	0.09	0.09
25	assign (segid 3A4 and resid 337 and name CA) (segid 3A4 and resid 339 and name CB)	7.99	0.10	0.11
	assign (segid 3A4 and resid 337 and name CA) (segid 3A4 and resid 339 and name N)	5.67	0.06	0.06
	assign (segid 3A4 and resid 337 and name CA) (segid 3A4 and resid 339 and name O)	7.48	0.13	0.13
	assign (segid 3A4 and resid 337 and name CA) (segid 3A4 and resid 340 and name CA)	8.61	0.09	0.09
	assign (segid 3A4 and resid 337 and name CA) (segid 3A4 and resid 340 and name N)	7.76	0.07	0.06
30	assign (segid 3A4 and resid 337 and name CA) (segid 3A4 and resid 341 and name C)	7.30	0.24	0.24
	assign (segid 3A4 and resid 337 and name CA) (segid 3A4 and resid 341 and name CA)	6.64	0.14	0.14
	assign (segid 3A4 and resid 337 and name CA) (segid 3A4 and resid 341 and name CB)	5.27	0.13	0.12
	assign (segid 3A4 and resid 337 and name CA) (segid 3A4 and resid 341 and name CG)	4.98	0.26	0.25
	assign (segid 3A4 and resid 337 and name CA) (segid 3A4 and resid 341 and name N)	6.85	0.13	0.13
35	assign (segid 3A4 and resid 337 and name CA) (segid 3A4 and resid 341 and name O)	7.32	0.35	0.34
	assign (segid 3A4 and resid 337 and name CA) (segid 3A4 and resid 342 and name CA)	9.01	0.30	0.31
	assign (segid 3A4 and resid 337 and name CA) (segid 3A4 and resid 342 and name CB)	9.05	0.44	0.44
	assign (segid 3A4 and resid 337 and name CA) (segid 3A4 and resid 343 and name CA)	8.40	0.54	0.55
	assign (segid 3A4 and resid 337 and name CA) (segid 3A4 and resid 344 and name CA)	12.50	0.54	0.54
40	assign (segid 3A4 and resid 337 and name CA) (segid 3A4 and resid 344 and name CB)	13.23	0.51	0.51
	assign (segid 3A4 and resid 337 and name CA) (segid 3A4 and resid 345 and name CA)	13.99	0.76	0.76
	assign (segid 3A4 and resid 337 and name CA) (segid 3A4 and resid 345 and name CB)	14.12	0.84	0.83
	assign (segid 3A4 and resid 337 and name CA) (segid 3A4 and resid 346 and name CA)	17.04	0.74	0.75
	assign (segid 3A4 and resid 337 and name CA) (segid 3A4 and resid 346 and name CB)	17.09	0.71	0.72
45	assign (segid 3A4 and resid 337 and name CA) (segid 3A4 and resid 338 and name C)	5.05	0.07	0.07
	assign (segid 3A4 and resid 337 and name CB) (segid 3A4 and resid 338 and name CA)	4.73	0.08	0.09
	assign (segid 3A4 and resid 337 and name CB) (segid 3A4 and resid 338 and name CB)	5.84	0.11	0.11
	assign (segid 3A4 and resid 337 and name CB) (segid 3A4 and resid 338 and name N)	3.46	0.12	0.12
	assign (segid 3A4 and resid 337 and name CB) (segid 3A4 and resid 338 and name O)	4.72	0.15	0.15
50	assign (segid 3A4 and resid 337 and name CB) (segid 3A4 and resid 339 and name C)	7.43	0.08	0.07
	assign (segid 3A4 and resid 337 and name CB) (segid 3A4 and resid 339 and name CA)	6.95	0.06	0.05
	assign (segid 3A4 and resid 337 and name CB) (segid 3A4 and resid 339 and name CB)	8.27	0.07	0.08
	assign (segid 3A4 and resid 337 and name CB) (segid 3A4 and resid 339 and name N)	6.12	0.06	0.05
	assign (segid 3A4 and resid 337 and name CB) (segid 3A4 and resid 340 and name CA)	8.49	0.18	0.17
55	assign (segid 3A4 and resid 337 and name CB) (segid 3A4 and resid 340 and name N)	7.67	0.15	0.14
	assign (segid 3A4 and resid 337 and name CB) (segid 3A4 and resid 341 and name C)	6.73	0.24	0.24
	assign (segid 3A4 and resid 337 and name CB) (segid 3A4 and resid 341 and name CA)	6.38	0.17	0.17
	assign (segid 3A4 and resid 337 and name CB) (segid 3A4 and resid 341 and name CB)	5.08	0.15	0.16
	assign (segid 3A4 and resid 337 and name CB) (segid 3A4 and resid 341 and name CG)	5.21	0.35	0.36
60	assign (segid 3A4 and resid 337 and name CB) (segid 3A4 and resid 341 and name N)	6.65	0.18	0.19
	assign (segid 3A4 and resid 337 and name CB) (segid 3A4 and resid 341 and name O)	6.57	0.33	0.33
	assign (segid 3A4 and resid 337 and name CB) (segid 3A4 and resid 342 and name CA)	8.25	0.33	0.33
	assign (segid 3A4 and resid 337 and name CB) (segid 3A4 and resid 342 and name N)	7.54	0.25	0.25
	assign (segid 3A4 and resid 337 and name CB) (segid 3A4 and resid 342 and name O)	7.38	0.43	0.44
65	assign (segid 3A4 and resid 337 and name CB) (segid 3A4 and resid 343 and name CA)	7.91	0.50	0.50
	assign (segid 3A4 and resid 337 and name CB) (segid 3A4 and resid 343 and name CB)	7.12	0.57	0.57
	assign (segid 3A4 and resid 337 and name CB) (segid 3A4 and resid 344 and name CA)	11.34	0.61	0.60
	assign (segid 3A4 and resid 337 and name CB) (segid 3A4 and resid 344 and name CB)	12.17	0.57	0.57
	assign (segid 3A4 and resid 337 and name CB) (segid 3A4 and resid 345 and name CA)	12.66	0.80	0.81
70	assign (segid 3A4 and resid 337 and name CB) (segid 3A4 and resid 345 and name CB)	12.72	0.87	0.87
	assign (segid 3A4 and resid 337 and name CB) (segid 3A4 and resid 346 and name CA)	15.82	0.79	0.78
	assign (segid 3A4 and resid 337 and name CB) (segid 3A4 and resid 346 and name CB)	15.95	0.73	0.72
	assign (segid 3A4 and resid 337 and name CB) (segid 3A4 and resid 347 and name CA)	18.34	0.76	0.76
	assign (segid 3A4 and resid 337 and name CB) (segid 3A4 and resid 349 and name CB)	18.10	0.75	0.76
75	assign (segid 3A4 and resid 337 and name CB) (segid 3A4 and resid 386 and name CA)	18.77	0.31	0.32
	assign (segid 3A4 and resid 337 and name CB) (segid 3A4 and resid 387 and name CA)	18.27	0.83	0.83
	assign (segid 3A4 and resid 337 and name CB) (segid 3A4 and resid 389 and name CB)	18.52	0.86	0.86
	assign (segid 3A4 and resid 337 and name CB) (segid 3A4 and resid 337 and name C)	2.41	0.03	0.03
	assign (segid 3A4 and resid 337 and name N) (segid 3A4 and resid 337 and name CA)	1.46	0.01	0.01
80	assign (segid 3A4 and resid 337 and name N) (segid 3A4 and resid 337 and name CB)	2.44	0.02	0.03
	assign (segid 3A4 and resid 337 and name N) (segid 3A4 and resid 337 and name O)	2.79	0.07	0.08
	assign (segid 3A4 and resid 337 and name N) (segid 3A4 and resid 338 and name C)	5.62	0.13	0.13

	assign (segid 3A4 and resid 337 and name N)	(segid 3A4 and resid 338 and name CA)	4.70	0.07	0.07
	assign (segid 3A4 and resid 337 and name N)	(segid 3A4 and resid 338 and name CB)	5.62	0.07	0.06
	assign (segid 3A4 and resid 337 and name N)	(segid 3A4 and resid 338 and name N)	3.45	0.06	0.06
	assign (segid 3A4 and resid 337 and name N)	(segid 3A4 and resid 338 and name O)	5.79	0.21	0.20
5	assign (segid 3A4 and resid 337 and name N)	(segid 3A4 and resid 339 and name N)	6.59	0.12	0.12
	assign (segid 3A4 and resid 337 and name N)	(segid 3A4 and resid 341 and name CB)	6.70	0.13	0.14
	assign (segid 3A4 and resid 337 and name N)	(segid 3A4 and resid 341 and name CG)	6.34	0.25	0.24
	assign (segid 3A4 and resid 337 and name N)	(segid 3A4 and resid 337 and name CB)	3.08	0.08	0.07
	assign (segid 3A4 and resid 337 and name O)	(segid 3A4 and resid 338 and name C)	3.38	0.25	0.24
	assign (segid 3A4 and resid 337 and name O)	(segid 3A4 and resid 338 and name CA)	2.78	0.03	0.03
10	assign (segid 3A4 and resid 337 and name O)	(segid 3A4 and resid 338 and name CB)	4.11	0.07	0.07
	assign (segid 3A4 and resid 337 and name O)	(segid 3A4 and resid 338 and name N)	2.24	0.01	0.01
	assign (segid 3A4 and resid 337 and name O)	(segid 3A4 and resid 338 and name O)	3.82	0.39	0.39
	assign (segid 3A4 and resid 337 and name O)	(segid 3A4 and resid 339 and name C)	6.09	0.28	0.27
	assign (segid 3A4 and resid 337 and name O)	(segid 3A4 and resid 339 and name CA)	5.17	0.29	0.30
15	assign (segid 3A4 and resid 337 and name O)	(segid 3A4 and resid 339 and name CB)	6.17	0.28	0.27
	assign (segid 3A4 and resid 337 and name O)	(segid 3A4 and resid 339 and name N)	4.06	0.21	0.20
	assign (segid 3A4 and resid 337 and name O)	(segid 3A4 and resid 339 and name O)	6.44	0.25	0.25
	assign (segid 3A4 and resid 337 and name O)	(segid 3A4 and resid 340 and name N)	6.75	0.26	0.26
20	assign (segid 3A4 and resid 337 and name O)	(segid 3A4 and resid 341 and name CA)	7.01	0.22	0.23
	assign (segid 3A4 and resid 337 and name O)	(segid 3A4 and resid 341 and name CB)	5.94	0.21	0.21
	assign (segid 3A4 and resid 337 and name O)	(segid 3A4 and resid 341 and name CG)	5.57	0.34	0.33
	assign (segid 3A4 and resid 337 and name O)	(segid 3A4 and resid 341 and name N)	6.72	0.22	0.22
	assign (segid 3A4 and resid 338 and name C)	(segid 3A4 and resid 338 and name CB)	2.48	0.04	0.05
25	assign (segid 3A4 and resid 338 and name C)	(segid 3A4 and resid 338 and name O)	1.24	0.01	0.01
	assign (segid 3A4 and resid 338 and name C)	(segid 3A4 and resid 339 and name C)	2.92	0.04	0.03
	assign (segid 3A4 and resid 338 and name C)	(segid 3A4 and resid 339 and name CA)	2.46	0.03	0.02
	assign (segid 3A4 and resid 338 and name C)	(segid 3A4 and resid 339 and name CB)	3.72	0.01	0.01
	assign (segid 3A4 and resid 338 and name C)	(segid 3A4 and resid 339 and name N)	1.33	0.00	0.01
	assign (segid 3A4 and resid 338 and name C)	(segid 3A4 and resid 339 and name O)	3.10	0.06	0.06
30	assign (segid 3A4 and resid 338 and name C)	(segid 3A4 and resid 340 and name C)	4.97	0.09	0.08
	assign (segid 3A4 and resid 338 and name C)	(segid 3A4 and resid 340 and name CA)	4.87	0.09	0.09
	assign (segid 3A4 and resid 338 and name C)	(segid 3A4 and resid 340 and name N)	3.81	0.10	0.10
	assign (segid 3A4 and resid 338 and name C)	(segid 3A4 and resid 340 and name O)	6.09	0.11	0.10
	assign (segid 3A4 and resid 338 and name C)	(segid 3A4 and resid 341 and name C)	6.02	0.17	0.18
35	assign (segid 3A4 and resid 338 and name C)	(segid 3A4 and resid 341 and name CA)	4.90	0.10	0.10
	assign (segid 3A4 and resid 338 and name C)	(segid 3A4 and resid 341 and name CB)	4.36	0.14	0.14
	assign (segid 3A4 and resid 338 and name C)	(segid 3A4 and resid 341 and name CG)	3.85	0.22	0.22
	assign (segid 3A4 and resid 338 and name C)	(segid 3A4 and resid 341 and name N)	4.16	0.11	0.11
	assign (segid 3A4 and resid 338 and name C)	(segid 3A4 and resid 341 and name O)	6.05	0.26	0.27
40	assign (segid 3A4 and resid 338 and name C)	(segid 3A4 and resid 342 and name N)	7.18	0.14	0.15
	assign (segid 3A4 and resid 338 and name C)	(segid 3A4 and resid 338 and name C)	1.52	0.01	0.01
	assign (segid 3A4 and resid 338 and name CA)	(segid 3A4 and resid 338 and name CB)	1.51	0.01	0.02
	assign (segid 3A4 and resid 338 and name CA)	(segid 3A4 and resid 338 and name O)	2.41	0.03	0.02
	assign (segid 3A4 and resid 338 and name CA)	(segid 3A4 and resid 339 and name C)	4.32	0.04	0.04
45	assign (segid 3A4 and resid 338 and name CA)	(segid 3A4 and resid 339 and name CA)	3.81	0.02	0.02
	assign (segid 3A4 and resid 338 and name CA)	(segid 3A4 and resid 339 and name CB)	4.83	0.01	0.02
	assign (segid 3A4 and resid 338 and name CA)	(segid 3A4 and resid 339 and name N)	2.42	0.02	0.02
	assign (segid 3A4 and resid 338 and name CA)	(segid 3A4 and resid 339 and name O)	4.24	0.11	0.11
50	assign (segid 3A4 and resid 338 and name CA)	(segid 3A4 and resid 340 and name C)	6.19	0.09	0.09
	assign (segid 3A4 and resid 338 and name CA)	(segid 3A4 and resid 340 and name CA)	6.25	0.07	0.08
	assign (segid 3A4 and resid 338 and name CA)	(segid 3A4 and resid 340 and name N)	5.29	0.09	0.08
	assign (segid 3A4 and resid 338 and name CA)	(segid 3A4 and resid 340 and name O)	7.22	0.13	0.14
	assign (segid 3A4 and resid 338 and name CA)	(segid 3A4 and resid 341 and name C)	6.94	0.20	0.19
	assign (segid 3A4 and resid 338 and name CA)	(segid 3A4 and resid 341 and name CA)	5.74	0.13	0.13
55	assign (segid 3A4 and resid 338 and name CA)	(segid 3A4 and resid 341 and name CB)	4.89	0.17	0.17
	assign (segid 3A4 and resid 338 and name CA)	(segid 3A4 and resid 341 and name CG)	4.07	0.16	0.17
	assign (segid 3A4 and resid 338 and name CA)	(segid 3A4 and resid 341 and name N)	5.29	0.13	0.12
	assign (segid 3A4 and resid 338 and name CA)	(segid 3A4 and resid 341 and name O)	7.08	0.29	0.30
	assign (segid 3A4 and resid 338 and name CA)	(segid 3A4 and resid 342 and name CA)	9.23	0.21	0.20
60	assign (segid 3A4 and resid 338 and name CA)	(segid 3A4 and resid 343 and name CA)	10.67	0.33	0.34
	assign (segid 3A4 and resid 338 and name CA)	(segid 3A4 and resid 343 and name CB)	10.28	0.42	0.43
	assign (segid 3A4 and resid 338 and name CA)	(segid 3A4 and resid 344 and name CA)	14.39	0.37	0.37
	assign (segid 3A4 and resid 338 and name CA)	(segid 3A4 and resid 344 and name CB)	15.04	0.36	0.36
	assign (segid 3A4 and resid 338 and name CA)	(segid 3A4 and resid 345 and name CA)	16.45	0.58	0.57
65	assign (segid 3A4 and resid 338 and name CA)	(segid 3A4 and resid 345 and name CB)	16.53	0.67	0.67
	assign (segid 3A4 and resid 338 and name CB)	(segid 3A4 and resid 339 and name C)	4.66	0.14	0.13
	assign (segid 3A4 and resid 338 and name CB)	(segid 3A4 and resid 339 and name CA)	4.49	0.09	0.10
	assign (segid 3A4 and resid 338 and name CB)	(segid 3A4 and resid 339 and name CB)	5.35	0.13	0.13
	assign (segid 3A4 and resid 338 and name CB)	(segid 3A4 and resid 339 and name N)	3.19	0.09	0.09
70	assign (segid 3A4 and resid 338 and name CB)	(segid 3A4 and resid 339 and name O)	4.17	0.20	0.20
	assign (segid 3A4 and resid 338 and name CB)	(segid 3A4 and resid 340 and name C)	6.34	0.18	0.19
	assign (segid 3A4 and resid 338 and name CB)	(segid 3A4 and resid 340 and name CA)	6.48	0.15	0.14
	assign (segid 3A4 and resid 338 and name CB)	(segid 3A4 and resid 340 and name N)	5.74	0.13	0.12
	assign (segid 3A4 and resid 338 and name CB)	(segid 3A4 and resid 340 and name O)	7.23	0.28	0.27
75	assign (segid 3A4 and resid 338 and name CB)	(segid 3A4 and resid 341 and name C)	7.31	0.19	0.19
	assign (segid 3A4 and resid 338 and name CB)	(segid 3A4 and resid 341 and name CA)	5.94	0.19	0.20
	assign (segid 3A4 and resid 338 and name CB)	(segid 3A4 and resid 341 and name CB)	5.16	0.24	0.24
	assign (segid 3A4 and resid 338 and name CB)	(segid 3A4 and resid 341 and name CG)	4.04	0.25	0.24
	assign (segid 3A4 and resid 338 and name CB)	(segid 3A4 and resid 341 and name N)	5.56	0.16	0.16
80	assign (segid 3A4 and resid 338 and name CB)	(segid 3A4 and resid 342 and name CA)	9.57	0.23	0.23
	assign (segid 3A4 and resid 338 and name CB)	(segid 3A4 and resid 343 and name CA)	11.32	0.43	0.43
	assign (segid 3A4 and resid 338 and name CB)	(segid 3A4 and resid 343 and name CB)	11.10	0.49	0.50

	assign (segid 3A4 and resid 338 and name CB)	(segid 3A4 and resid 344 and name CA)	14.98	0.19	0.49
	assign (segid 3A4 and resid 338 and name CB)	(segid 3A4 and resid 344 and name CB)	15.51	0.51	0.50
	assign (segid 3A4 and resid 338 and name CB)	(segid 3A4 and resid 345 and name CA)	17.26	0.63	0.64
	assign (segid 3A4 and resid 338 and name CB)	(segid 3A4 and resid 345 and name CB)	17.45	0.68	0.67
5	assign (segid 3A4 and resid 338 and name N)	(segid 3A4 and resid 338 and name C)	2.48	0.04	0.04
	assign (segid 3A4 and resid 338 and name N)	(segid 3A4 and resid 338 and name CA)	1.46	0.00	0.01
	assign (segid 3A4 and resid 338 and name N)	(segid 3A4 and resid 338 and name CB)	2.42	0.06	0.05
	assign (segid 3A4 and resid 338 and name N)	(segid 3A4 and resid 338 and name O)	2.80	0.07	0.08
	assign (segid 3A4 and resid 338 and name N)	(segid 3A4 and resid 339 and name C)	5.32	0.07	0.06
10	assign (segid 3A4 and resid 338 and name N)	(segid 3A4 and resid 339 and name CA)	4.89	0.03	0.03
	assign (segid 3A4 and resid 338 and name N)	(segid 3A4 and resid 339 and name CB)	6.07	0.03	0.03
	assign (segid 3A4 and resid 338 and name N)	(segid 3A4 and resid 339 and name N)	3.63	0.03	0.03
	assign (segid 3A4 and resid 338 and name N)	(segid 3A4 and resid 339 and name O)	5.32	0.13	0.13
	assign (segid 3A4 and resid 338 and name N)	(segid 3A4 and resid 340 and name C)	6.62	0.14	0.14
15	assign (segid 3A4 and resid 338 and name N)	(segid 3A4 and resid 340 and name CA)	6.94	0.13	0.13
	assign (segid 3A4 and resid 338 and name N)	(segid 3A4 and resid 340 and name N)	6.07	0.14	0.13
	assign (segid 3A4 and resid 338 and name N)	(segid 3A4 and resid 340 and name O)	7.59	0.12	0.13
	assign (segid 3A4 and resid 338 and name N)	(segid 3A4 and resid 341 and name C)	6.69	0.25	0.24
	assign (segid 3A4 and resid 338 and name N)	(segid 3A4 and resid 341 and name CA)	5.63	0.17	0.18
20	assign (segid 3A4 and resid 338 and name N)	(segid 3A4 and resid 341 and name CB)	4.48	0.18	0.18
	assign (segid 3A4 and resid 338 and name N)	(segid 3A4 and resid 341 and name CG)	3.77	0.17	0.16
	assign (segid 3A4 and resid 338 and name N)	(segid 3A4 and resid 341 and name N)	5.51	0.19	0.18
	assign (segid 3A4 and resid 338 and name N)	(segid 3A4 and resid 341 and name O)	6.85	0.35	0.36
	assign (segid 3A4 and resid 338 and name O)	(segid 3A4 and resid 338 and name CB)	3.24	0.07	0.07
25	assign (segid 3A4 and resid 338 and name O)	(segid 3A4 and resid 339 and name C)	2.81	0.09	0.10
	assign (segid 3A4 and resid 338 and name O)	(segid 3A4 and resid 339 and name CA)	2.79	0.02	0.03
	assign (segid 3A4 and resid 338 and name O)	(segid 3A4 and resid 339 and name CB)	4.27	0.01	0.02
	assign (segid 3A4 and resid 338 and name O)	(segid 3A4 and resid 339 and name N)	2.25	0.00	0.01
	assign (segid 3A4 and resid 338 and name O)	(segid 3A4 and resid 339 and name O)	3.12	0.10	0.10
30	assign (segid 3A4 and resid 338 and name O)	(segid 3A4 and resid 340 and name C)	4.07	0.16	0.16
	assign (segid 3A4 and resid 338 and name O)	(segid 3A4 and resid 340 and name CA)	4.22	0.18	0.18
	assign (segid 3A4 and resid 338 and name O)	(segid 3A4 and resid 340 and name N)	3.32	0.16	0.17
	assign (segid 3A4 and resid 338 and name O)	(segid 3A4 and resid 340 and name O)	5.19	0.15	0.14
	assign (segid 3A4 and resid 338 and name O)	(segid 3A4 and resid 341 and name C)	4.83	0.20	0.19
35	assign (segid 3A4 and resid 338 and name O)	(segid 3A4 and resid 341 and name CA)	3.77	0.12	0.12
	assign (segid 3A4 and resid 338 and name O)	(segid 3A4 and resid 341 and name CB)	3.28	0.11	0.11
	assign (segid 3A4 and resid 338 and name O)	(segid 3A4 and resid 341 and name CG)	3.05	0.27	0.27
	assign (segid 3A4 and resid 338 and name O)	(segid 3A4 and resid 341 and name N)	3.10	0.17	0.17
	assign (segid 3A4 and resid 338 and name O)	(segid 3A4 and resid 341 and name O)	4.85	0.29	0.29
40	assign (segid 3A4 and resid 338 and name O)	(segid 3A4 and resid 342 and name C)	7.59	0.20	0.21
	assign (segid 3A4 and resid 338 and name O)	(segid 3A4 and resid 342 and name CA)	7.20	0.19	0.19
	assign (segid 3A4 and resid 338 and name O)	(segid 3A4 and resid 342 and name N)	6.00	0.16	0.16
	assign (segid 3A4 and resid 339 and name C)	(segid 3A4 and resid 339 and name CB)	2.50	0.01	0.01
45	assign (segid 3A4 and resid 339 and name C)	(segid 3A4 and resid 339 and name O)	1.23	0.00	0.01
	assign (segid 3A4 and resid 339 and name C)	(segid 3A4 and resid 340 and name C)	3.29	0.06	0.06
	assign (segid 3A4 and resid 339 and name C)	(segid 3A4 and resid 340 and name CA)	2.44	0.02	0.01
	assign (segid 3A4 and resid 339 and name C)	(segid 3A4 and resid 340 and name N)	1.33	0.01	0.00
	assign (segid 3A4 and resid 339 and name C)	(segid 3A4 and resid 340 and name O)	4.40	0.10	0.11
50	assign (segid 3A4 and resid 339 and name C)	(segid 3A4 and resid 341 and name C)	5.65	0.09	0.10
	assign (segid 3A4 and resid 339 and name C)	(segid 3A4 and resid 341 and name CA)	4.67	0.09	0.08
	assign (segid 3A4 and resid 339 and name C)	(segid 3A4 and resid 341 and name CB)	5.04	0.14	0.14
	assign (segid 3A4 and resid 339 and name C)	(segid 3A4 and resid 341 and name CG)	4.91	0.26	0.26
	assign (segid 3A4 and resid 339 and name C)	(segid 3A4 and resid 341 and name N)	3.30	0.05	0.06
	assign (segid 3A4 and resid 339 and name C)	(segid 3A4 and resid 341 and name O)	5.59	0.13	0.13
55	assign (segid 3A4 and resid 339 and name C)	(segid 3A4 and resid 342 and name N)	6.83	0.07	0.07
	assign (segid 3A4 and resid 339 and name CA)	(segid 3A4 and resid 339 and name C)	1.53	0.01	0.00
	assign (segid 3A4 and resid 339 and name CA)	(segid 3A4 and resid 339 and name CB)	1.54	0.02	0.01
	assign (segid 3A4 and resid 339 and name CA)	(segid 3A4 and resid 339 and name O)	2.40	0.02	0.02
	assign (segid 3A4 and resid 339 and name CA)	(segid 3A4 and resid 340 and name C)	4.63	0.04	0.05
60	assign (segid 3A4 and resid 339 and name CA)	(segid 3A4 and resid 340 and name CA)	3.80	0.03	0.04
	assign (segid 3A4 and resid 339 and name CA)	(segid 3A4 and resid 340 and name N)	2.43	0.04	0.03
	assign (segid 3A4 and resid 339 and name CA)	(segid 3A4 and resid 340 and name O)	5.81	0.09	0.08
	assign (segid 3A4 and resid 339 and name CA)	(segid 3A4 and resid 341 and name C)	6.57	0.11	0.11
	assign (segid 3A4 and resid 339 and name CA)	(segid 3A4 and resid 341 and name CA)	5.65	0.07	0.08
65	assign (segid 3A4 and resid 339 and name CA)	(segid 3A4 and resid 341 and name CB)	5.72	0.14	0.14
	assign (segid 3A4 and resid 339 and name CA)	(segid 3A4 and resid 341 and name CG)	5.54	0.28	0.28
	assign (segid 3A4 and resid 339 and name CA)	(segid 3A4 and resid 341 and name N)	4.39	0.04	0.05
	assign (segid 3A4 and resid 339 and name CA)	(segid 3A4 and resid 341 and name O)	6.35	0.17	0.17
	assign (segid 3A4 and resid 339 and name CA)	(segid 3A4 and resid 342 and name CA)	8.94	0.12	0.13
70	assign (segid 3A4 and resid 339 and name CA)	(segid 3A4 and resid 342 and name N)	7.83	0.10	0.09
	assign (segid 3A4 and resid 339 and name CA)	(segid 3A4 and resid 343 and name CA)	11.01	0.25	0.24
	assign (segid 3A4 and resid 339 and name CA)	(segid 3A4 and resid 343 and name CB)	10.61	0.35	0.34
	assign (segid 3A4 and resid 339 and name CA)	(segid 3A4 and resid 344 and name CA)	14.74	0.20	0.20
	assign (segid 3A4 and resid 339 and name CA)	(segid 3A4 and resid 344 and name CB)	15.53	0.19	0.19
75	assign (segid 3A4 and resid 339 and name CA)	(segid 3A4 and resid 345 and name CA)	16.85	0.40	0.40
	assign (segid 3A4 and resid 339 and name CA)	(segid 3A4 and resid 345 and name CB)	16.71	0.53	0.53
	assign (segid 3A4 and resid 339 and name CB)	(segid 3A4 and resid 340 and name C)	5.72	0.06	0.07
	assign (segid 3A4 and resid 339 and name CB)	(segid 3A4 and resid 340 and name CA)	4.62	0.04	0.03
	assign (segid 3A4 and resid 339 and name CB)	(segid 3A4 and resid 340 and name N)	3.36	0.06	0.06
80	assign (segid 3A4 and resid 339 and name CB)	(segid 3A4 and resid 340 and name O)	6.82	0.11	0.10
	assign (segid 3A4 and resid 339 and name CB)	(segid 3A4 and resid 341 and name CA)	7.05	0.08	0.08
	assign (segid 3A4 and resid 339 and name CB)	(segid 3A4 and resid 341 and name CB)	7.20	0.14	0.14
	assign (segid 3A4 and resid 339 and name CB)	(segid 3A4 and resid 341 and name CG)	6.95	0.26	0.25

	assign (segid 3A4 and resid 339 and name CB)	(segid 3A4 and resid 341 and name N)	5.72	0.06	0.06
	assign (segid 3A4 and resid 339 and name CB)	(segid 3A4 and resid 341 and name O)	7.72	0.14	0.14
	assign (segid 3A4 and resid 339 and name CB)	(segid 3A4 and resid 342 and name CA)	10.31	0.10	0.10
	assign (segid 3A4 and resid 339 and name CB)	(segid 3A4 and resid 343 and name CA)	12.46	0.25	0.25
	assign (segid 3A4 and resid 339 and name CB)	(segid 3A4 and resid 343 and name CB)	12.04	0.35	0.35
5	assign (segid 3A4 and resid 339 and name CB)	(segid 3A4 and resid 344 and name CA)	16.18	0.20	0.19
	assign (segid 3A4 and resid 339 and name CB)	(segid 3A4 and resid 344 and name CB)	16.98	0.19	0.19
	assign (segid 3A4 and resid 339 and name CB)	(segid 3A4 and resid 345 and name CA)	18.25	0.40	0.39
	assign (segid 3A4 and resid 339 and name CB)	(segid 3A4 and resid 345 and name CB)	18.05	0.51	0.52
	assign (segid 3A4 and resid 339 and name CB)	(segid 3A4 and resid 339 and name C)	2.42	0.03	0.03
10	assign (segid 3A4 and resid 339 and name N)	(segid 3A4 and resid 339 and name CA)	1.46	0.00	0.01
	assign (segid 3A4 and resid 339 and name N)	(segid 3A4 and resid 339 and name CB)	2.45	0.01	0.01
	assign (segid 3A4 and resid 339 and name N)	(segid 3A4 and resid 339 and name O)	2.77	0.07	0.08
	assign (segid 3A4 and resid 339 and name N)	(segid 3A4 and resid 340 and name C)	5.24	0.06	0.07
	assign (segid 3A4 and resid 339 and name N)	(segid 3A4 and resid 340 and name CA)	4.75	0.04	0.04
15	assign (segid 3A4 and resid 339 and name N)	(segid 3A4 and resid 340 and name N)	3.51	0.05	0.04
	assign (segid 3A4 and resid 339 and name N)	(segid 3A4 and resid 340 and name O)	6.40	0.12	0.12
	assign (segid 3A4 and resid 339 and name N)	(segid 3A4 and resid 341 and name C)	6.81	0.14	0.14
	assign (segid 3A4 and resid 339 and name N)	(segid 3A4 and resid 341 and name CA)	5.73	0.09	0.09
	assign (segid 3A4 and resid 339 and name N)	(segid 3A4 and resid 341 and name CB)	5.45	0.15	0.14
20	assign (segid 3A4 and resid 339 and name N)	(segid 3A4 and resid 341 and name CG)	4.99	0.23	0.24
	assign (segid 3A4 and resid 339 and name N)	(segid 3A4 and resid 341 and name N)	4.72	0.08	0.07
	assign (segid 3A4 and resid 339 and name N)	(segid 3A4 and resid 341 and name O)	6.72	0.22	0.23
	assign (segid 3A4 and resid 339 and name O)	(segid 3A4 and resid 339 and name CB)	3.11	0.07	0.08
	assign (segid 3A4 and resid 339 and name O)	(segid 3A4 and resid 340 and name C)	3.39	0.12	0.11
25	assign (segid 3A4 and resid 339 and name O)	(segid 3A4 and resid 340 and name CA)	2.78	0.03	0.03
	assign (segid 3A4 and resid 339 and name O)	(segid 3A4 and resid 340 and name N)	2.25	0.02	0.01
	assign (segid 3A4 and resid 339 and name O)	(segid 3A4 and resid 340 and name O)	4.33	0.20	0.19
	assign (segid 3A4 and resid 339 and name O)	(segid 3A4 and resid 340 and name C)	5.89	0.12	0.12
	assign (segid 3A4 and resid 339 and name O)	(segid 3A4 and resid 341 and name CA)	4.69	0.16	0.15
30	assign (segid 3A4 and resid 339 and name O)	(segid 3A4 and resid 341 and name CB)	5.04	0.24	0.25
	assign (segid 3A4 and resid 339 and name O)	(segid 3A4 and resid 341 and name CG)	4.63	0.31	0.30
	assign (segid 3A4 and resid 339 and name O)	(segid 3A4 and resid 341 and name N)	3.47	0.10	0.10
	assign (segid 3A4 and resid 339 and name O)	(segid 3A4 and resid 341 and name O)	6.07	0.13	0.14
	assign (segid 3A4 and resid 339 and name O)	(segid 3A4 and resid 342 and name N)	6.95	0.10	0.09
35	assign (segid 3A4 and resid 339 and name O)	(segid 3A4 and resid 33 and name CB)	2.51	0.04	0.04
	assign (segid 3A4 and resid 33 and name C)	(segid 3A4 and resid 33 and name O)	1.24	0.01	0.00
	assign (segid 3A4 and resid 33 and name C)	(segid 3A4 and resid 344 and name C)	5.52	0.13	0.14
	assign (segid 3A4 and resid 33 and name C)	(segid 3A4 and resid 344 and name CA)	6.80	0.13	0.12
	assign (segid 3A4 and resid 33 and name C)	(segid 3A4 and resid 344 and name CB)	7.15	0.23	0.24
40	assign (segid 3A4 and resid 33 and name C)	(segid 3A4 and resid 344 and name N)	6.98	0.16	0.17
	assign (segid 3A4 and resid 33 and name C)	(segid 3A4 and resid 344 and name O)	4.47	0.12	0.12
	assign (segid 3A4 and resid 33 and name C)	(segid 3A4 and resid 345 and name C)	5.30	0.33	0.34
	assign (segid 3A4 and resid 33 and name C)	(segid 3A4 and resid 345 and name CA)	5.01	0.27	0.27
	assign (segid 3A4 and resid 33 and name C)	(segid 3A4 and resid 345 and name CB)	5.89	0.38	0.38
45	assign (segid 3A4 and resid 33 and name C)	(segid 3A4 and resid 345 and name N)	5.78	0.18	0.17
	assign (segid 3A4 and resid 33 and name C)	(segid 3A4 and resid 345 and name O)	6.48	0.31	0.32
	assign (segid 3A4 and resid 33 and name C)	(segid 3A4 and resid 346 and name C)	5.90	0.49	0.49
	assign (segid 3A4 and resid 33 and name C)	(segid 3A4 and resid 346 and name CA)	5.34	0.50	0.51
	assign (segid 3A4 and resid 33 and name C)	(segid 3A4 and resid 346 and name CB)	4.92	0.49	0.50
50	assign (segid 3A4 and resid 33 and name C)	(segid 3A4 and resid 346 and name N)	4.51	0.42	0.43
	assign (segid 3A4 and resid 33 and name C)	(segid 3A4 and resid 346 and name O)	5.59	0.44	0.43
	assign (segid 3A4 and resid 33 and name C)	(segid 3A4 and resid 349 and name CA)	7.22	0.31	0.32
	assign (segid 3A4 and resid 33 and name C)	(segid 3A4 and resid 349 and name CB)	5.96	0.24	0.24
	assign (segid 3A4 and resid 33 and name C)	(segid 3A4 and resid 34 and name C)	3.51	0.09	0.08
55	assign (segid 3A4 and resid 33 and name C)	(segid 3A4 and resid 34 and name CA)	2.44	0.02	0.02
	assign (segid 3A4 and resid 33 and name C)	(segid 3A4 and resid 34 and name CB)	3.51	0.06	0.05
	assign (segid 3A4 and resid 33 and name C)	(segid 3A4 and resid 34 and name N)	1.33	0.01	0.01
	assign (segid 3A4 and resid 33 and name C)	(segid 3A4 and resid 34 and name O)	4.48	0.09	0.10
	assign (segid 3A4 and resid 33 and name C)	(segid 3A4 and resid 35 and name C)	5.58	0.15	0.15
60	assign (segid 3A4 and resid 33 and name C)	(segid 3A4 and resid 35 and name CA)	5.22	0.17	0.18
	assign (segid 3A4 and resid 33 and name C)	(segid 3A4 and resid 35 and name N)	3.86	0.18	0.18
	assign (segid 3A4 and resid 33 and name C)	(segid 3A4 and resid 35 and name O)	5.04	0.16	0.16
	assign (segid 3A4 and resid 33 and name C)	(segid 3A4 and resid 36 and name CA)	7.56	0.15	0.15
	assign (segid 3A4 and resid 33 and name C)	(segid 3A4 and resid 36 and name N)	6.80	0.17	0.17
65	assign (segid 3A4 and resid 33 and name C)	(segid 3A4 and resid 38 and name C)	6.21	0.36	0.35
	assign (segid 3A4 and resid 33 and name C)	(segid 3A4 and resid 38 and name CA)	6.48	0.34	0.35
	assign (segid 3A4 and resid 33 and name C)	(segid 3A4 and resid 38 and name CB)	5.51	0.38	0.38
	assign (segid 3A4 and resid 33 and name C)	(segid 3A4 and resid 38 and name N)	7.03	0.26	0.25
	assign (segid 3A4 and resid 33 and name C)	(segid 3A4 and resid 38 and name O)	6.73	0.41	0.41
70	assign (segid 3A4 and resid 33 and name C)	(segid 3A4 and resid 39 and name C)	7.46	0.29	0.30
	assign (segid 3A4 and resid 33 and name C)	(segid 3A4 and resid 39 and name CA)	5.97	0.29	0.29
	assign (segid 3A4 and resid 33 and name C)	(segid 3A4 and resid 39 and name CB)	5.69	0.23	0.24
	assign (segid 3A4 and resid 33 and name C)	(segid 3A4 and resid 39 and name N)	5.76	0.28	0.29
	assign (segid 3A4 and resid 33 and name CA)	(segid 3A4 and resid 314 and name CA)	17.27	0.55	0.56
75	assign (segid 3A4 and resid 33 and name CA)	(segid 3A4 and resid 314 and name CB)	17.76	0.50	0.50
	assign (segid 3A4 and resid 33 and name CA)	(segid 3A4 and resid 315 and name CA)	18.24	0.79	0.78
	assign (segid 3A4 and resid 33 and name CA)	(segid 3A4 and resid 317 and name CA)	15.63	0.40	0.40
	assign (segid 3A4 and resid 33 and name CA)	(segid 3A4 and resid 318 and name CA)	17.05	0.60	0.59
	assign (segid 3A4 and resid 33 and name CA)	(segid 3A4 and resid 318 and name CB)	18.36	0.53	0.53
80	assign (segid 3A4 and resid 33 and name CA)	(segid 3A4 and resid 319 and name CA)	14.70	0.56	0.57
	assign (segid 3A4 and resid 33 and name CA)	(segid 3A4 and resid 319 and name CB)	14.94	0.69	0.70
	assign (segid 3A4 and resid 33 and name CA)	(segid 3A4 and resid 322 and name CA)	10.29	0.51	0.52

	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 323 and name CA)	10.84	0.25	0.26
	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 323 and name CB)	10.12	0.41	0.42
	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 324 and name CA)	12.66	0.29	0.28
	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 324 and name CB)	14.05	0.32	0.32
5	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 325 and name CA)	13.16	0.27	0.27
	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 325 and name CB)	12.71	0.32	0.33
	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 326 and name CA)	16.80	0.24	0.24
	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 326 and name CB)	17.39	0.25	0.25
	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 327 and name CA)	17.50	0.36	0.35
10	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 327 and name CB)	18.22	0.46	0.46
	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 328 and name CA)	16.32	0.57	0.58
	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 328 and name CB)	17.36	0.63	0.64
	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 329 and name CA)	14.00	0.75	0.75
	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 329 and name CB)	13.22	0.81	0.81
15	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 330 and name CA)	12.92	0.70	0.71
	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 330 and name CB)	14.16	0.73	0.72
	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 331 and name CA)	9.72	0.70	0.70
	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 331 and name CB)	8.46	0.71	0.71
	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 332 and name CA)	10.33	0.76	0.76
20	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 332 and name CB)	12.94	0.87	0.88
	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 335 and name CA)	11.19	0.59	0.59
	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 335 and name CB)	13.01	0.52	0.51
	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 336 and name CA)	14.44	0.49	0.50
	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 336 and name CB)	11.78	0.62	0.63
25	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 337 and name CA)	10.70	0.63	0.63
	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 338 and name CA)	14.97	0.49	0.49
	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 338 and name CB)	15.71	0.59	0.59
	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 339 and name CA)	16.48	0.35	0.34
	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 339 and name CB)	17.95	0.37	0.37
30	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 33 and name C)	1.53	0.01	0.01
	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 33 and name CB)	1.53	0.02	0.02
	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 33 and name O)	2.40	0.02	0.01
	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 340 and name CA)	16.04	0.17	0.17
	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 341 and name CA)	12.79	0.19	0.18
35	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 341 and name CB)	12.05	0.28	0.28
	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 342 and name CA)	10.86	0.15	0.14
	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 343 and name C)	7.04	0.19	0.19
	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 343 and name CA)	7.24	0.19	0.19
	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 343 and name CB)	6.92	0.23	0.24
40	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 344 and name C)	5.18	0.12	0.11
	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 344 and name CA)	6.31	0.14	0.14
	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 344 and name CB)	6.81	0.24	0.24
	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 344 and name N)	6.20	0.18	0.17
	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 344 and name O)	4.08	0.09	0.08
45	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 345 and name C)	5.76	0.25	0.26
	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 345 and name CA)	5.09	0.19	0.19
	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 345 and name CB)	5.90	0.27	0.27
	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 345 and name N)	5.62	0.15	0.14
	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 345 and name O)	6.97	0.23	0.22
50	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 346 and name C)	7.01	0.39	0.40
	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 346 and name CA)	6.32	0.43	0.42
	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 346 and name CB)	6.03	0.45	0.45
	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 346 and name N)	5.25	0.35	0.36
	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 346 and name O)	6.84	0.33	0.34
55	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 347 and name CA)	9.06	0.40	0.40
	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 347 and name CB)	10.24	0.43	0.43
	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 348 and name CA)	10.85	0.29	0.30
	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 349 and name CA)	8.72	0.30	0.30
	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 349 and name CB)	7.45	0.24	0.24
60	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 34 and name C)	4.79	0.09	0.08
	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 34 and name CA)	3.80	0.02	0.03
	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 34 and name CB)	4.69	0.04	0.04
	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 34 and name N)	2.43	0.03	0.02
	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 34 and name O)	5.86	0.09	0.09
65	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 350 and name CA)	8.94	0.73	0.72
	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 350 and name CB)	8.75	0.85	0.85
	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 351 and name CA)	12.55	0.60	0.60
	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 352 and name CA)	13.10	0.61	0.61
	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 352 and name CB)	13.06	0.63	0.64
70	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 353 and name CA)	11.94	0.74	0.74
	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 353 and name CB)	11.13	0.85	0.86
	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 354 and name CA)	15.24	0.74	0.73
	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 354 and name CB)	15.68	0.70	0.70
	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 355 and name CA)	15.26	1.11	1.11
75	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 355 and name CB)	14.39	1.26	1.26
	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 356 and name CA)	15.53	0.87	0.86
	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 356 and name CB)	14.42	0.82	0.81
	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 357 and name CA)	17.47	0.78	0.77
	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 357 and name CB)	17.02	0.77	0.78
80	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 35 and name C)	6.45	0.17	0.16
	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 35 and name CA)	6.14	0.21	0.21
	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 35 and name N)	4.84	0.20	0.19
	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 35 and name O)	5.75	0.12	0.12

	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 360 and name CA)	17.87	0.56	0.56
	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 360 and name CB)	16.47	0.57	0.57
	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 36 and name CA)	8.42	0.12	0.12
	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 36 and name N)	7.72	0.17	0.16
	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 37 and name CA)	9.23	0.16	0.17
5	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 37 and name CB)	9.83	0.21	0.22
	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 381 and name CA)	15.14	0.62	0.62
	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 382 and name CA)	13.16	0.42	0.41
	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 382 and name CB)	11.73	0.43	0.44
	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 383 and name CA)	14.95	0.31	0.32
10	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 384 and name CA)	16.53	0.32	0.32
	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 384 and name CB)	17.84	0.35	0.35
	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 385 and name CA)	13.64	0.51	0.50
	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 386 and name CA)	13.95	0.42	0.43
	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 387 and name CA)	15.57	1.13	1.13
15	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 389 and name CA)	17.27	0.74	0.73
	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 389 and name CB)	16.32	0.73	0.74
	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 38 and name C)	5.98	0.30	0.30
	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 38 and name CA)	6.26	0.30	0.29
	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 38 and name CB)	5.19	0.30	0.30
20	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 38 and name N)	7.08	0.22	0.21
	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 38 and name O)	6.27	0.39	0.38
	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 390 and name CA)	17.38	0.70	0.69
	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 390 and name CB)	17.81	0.74	0.75
	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 391 and name CB)	19.40	0.39	0.39
25	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 39 and name C)	7.50	0.26	0.25
	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 39 and name CA)	6.07	0.24	0.25
	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 39 and name CB)	6.15	0.21	0.22
	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 39 and name N)	5.83	0.22	0.23
	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 40 and name CA)	9.81	0.24	0.24
30	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 40 and name CB)	10.79	0.22	0.22
	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 41 and name CA)	9.98	0.20	0.21
	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 41 and name CB)	9.62	0.23	0.23
	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 42 and name CA)	8.44	0.24	0.24
	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 42 and name CB)	7.07	0.25	0.24
35	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 431 and name CA)	16.38	1.35	1.36
	assign (segid 3A4 and resid 33 and name CA) (segid 3A4 and resid 433 and name CA)	18.71	0.61	0.61
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 314 and name CA)	17.21	0.54	0.54
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 314 and name CB)	17.68	0.49	0.49
40	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 317 and name CA)	15.72	0.43	0.43
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 318 and name CA)	17.12	0.63	0.64
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 318 and name CB)	18.38	0.61	0.60
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 319 and name CA)	14.63	0.66	0.67
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 319 and name CB)	14.72	0.82	0.82
45	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 322 and name CA)	9.74	0.55	0.55
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 323 and name CA)	9.97	0.35	0.34
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 323 and name CB)	9.10	0.49	0.49
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 324 and name CA)	11.86	0.33	0.33
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 324 and name CB)	13.30	0.35	0.36
50	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 325 and name CA)	12.25	0.30	0.30
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 325 and name CB)	11.88	0.35	0.34
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 326 and name CA)	15.78	0.25	0.26
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 326 and name CB)	16.29	0.26	0.25
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 327 and name CA)	16.56	0.36	0.35
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 327 and name CB)	17.21	0.46	0.45
55	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 328 and name CA)	15.55	0.61	0.61
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 328 and name CB)	16.66	0.68	0.67
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 329 and name CA)	13.12	0.82	0.82
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 329 and name CB)	12.24	0.87	0.86
60	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 330 and name CA)	12.21	0.80	0.80
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 330 and name CB)	13.48	0.82	0.82
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 331 and name CA)	8.97	0.81	0.81
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 331 and name CB)	7.66	0.83	0.83
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 332 and name CA)	9.90	0.79	0.79
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 333 and name CA)	12.72	0.87	0.87
65	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 335 and name CA)	11.13	0.66	0.66
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 336 and name CA)	12.70	0.63	0.63
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 336 and name CB)	14.18	0.62	0.62
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 337 and name CA)	11.38	0.65	0.65
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 337 and name CB)	10.17	0.65	0.66
70	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 338 and name CA)	14.55	0.49	0.48
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 338 and name CB)	15.40	0.56	0.56
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 339 and name CA)	15.83	0.33	0.33
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 339 and name CB)	17.27	0.36	0.35
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 340 and name CA)	15.50	0.23	0.23
75	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 341 and name CA)	12.46	0.22	0.23
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 341 and name CB)	11.76	0.29	0.29
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 342 and name CA)	10.58	0.22	0.22
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 343 and name C)	6.69	0.27	0.27
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 343 and name CA)	6.87	0.25	0.25
80	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 343 and name CB)	6.28	0.26	0.26
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 343 and name O)	7.38	0.31	0.31
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 344 and name C)	5.05	0.19	0.19

	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 344 and name CA)	6.24	0.23	0.24
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 344 and name CB)	7.06	0.29	0.28
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 344 and name N)	6.07	0.28	0.27
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 344 and name O)	4.16	0.18	0.18
5	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 345 and name C)	5.56	0.22	0.22
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 345 and name CA)	4.62	0.16	0.16
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 345 and name CB)	5.09	0.21	0.21
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 345 and name N)	5.25	0.18	0.18
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 345 and name O)	6.71	0.17	0.18
10	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 346 and name C)	7.11	0.32	0.33
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 346 and name CA)	6.57	0.36	0.36
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 346 and name CB)	6.63	0.39	0.38
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 346 and name N)	5.34	0.32	0.31
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 346 and name O)	7.00	0.23	0.23
15	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 347 and name CA)	8.90	0.34	0.34
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 347 and name CB)	9.96	0.37	0.37
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 348 and name CA)	11.16	0.26	0.27
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 349 and name CA)	9.28	0.25	0.25
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 349 and name CB)	8.17	0.19	0.19
20	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 34 and name C)	5.38	0.09	0.09
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 34 and name CA)	4.72	0.05	0.06
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 34 and name CB)	5.86	0.09	0.08
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 34 and name N)	3.44	0.08	0.07
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 34 and name O)	6.41	0.06	0.05
25	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 350 and name CA)	8.95	0.67	0.67
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 350 and name CB)	8.52	0.78	0.78
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 351 and name CA)	12.58	0.55	0.55
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 352 and name CA)	13.52	0.59	0.58
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 352 and name CB)	13.62	0.62	0.62
30	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 353 and name CA)	12.29	0.75	0.74
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 353 and name CB)	11.34	0.87	0.87
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 354 and name CA)	15.65	0.78	0.77
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 354 and name CB)	16.20	0.73	0.74
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 355 and name CA)	15.39	1.18	1.19
35	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 355 and name CB)	14.49	1.34	1.34
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 356 and name CA)	15.42	0.94	0.93
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 356 and name CB)	14.23	0.88	0.88
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 357 and name CA)	17.53	0.81	0.81
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 357 and name CB)	17.11	0.78	0.78
40	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 35 and name C)	6.30	0.24	0.23
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 35 and name CA)	6.32	0.28	0.27
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 35 and name N)	5.22	0.27	0.27
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 35 and name O)	5.38	0.21	0.22
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 360 and name CA)	18.31	0.56	0.55
45	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 360 and name CB)	16.93	0.58	0.58
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 36 and name CA)	8.00	0.16	0.16
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 37 and name C)	7.45	0.22	0.22
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 37 and name CA)	8.53	0.18	0.18
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 37 and name CB)	9.26	0.27	0.27
50	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 381 and name CA)	14.63	0.66	0.66
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 382 and name CA)	12.49	0.45	0.45
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 382 and name CB)	11.03	0.45	0.45
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 383 and name CA)	14.49	0.39	0.40
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 384 and name CA)	15.80	0.41	0.42
55	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 384 and name CB)	17.07	0.44	0.44
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 385 and name CA)	12.72	0.56	0.57
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 386 and name CA)	12.77	0.48	0.47
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 387 and name CA)	14.21	1.17	1.16
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 388 and name CA)	16.90	1.09	1.09
60	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 388 and name CB)	17.28	1.25	1.24
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 389 and name CA)	16.07	0.80	0.79
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 389 and name CB)	15.16	0.80	0.79
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 38 and name C)	4.84	0.24	0.23
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 38 and name CA)	5.35	0.26	0.26
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 38 and name CB)	4.51	0.30	0.30
65	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 38 and name N)	6.32	0.23	0.22
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 38 and name O)	4.96	0.33	0.34
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 390 and name CA)	16.26	0.75	0.76
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 390 and name CB)	16.67	0.79	0.78
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 391 and name CA)	18.56	0.61	0.61
70	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 391 and name CB)	18.56	0.49	0.50
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 39 and name C)	6.24	0.24	0.23
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 39 and name CA)	4.91	0.21	0.20
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 39 and name CB)	5.22	0.25	0.26
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 39 and name N)	4.77	0.17	0.17
75	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 39 and name O)	6.56	0.31	0.30
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 40 and name CA)	8.56	0.20	0.21
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 40 and name CB)	9.63	0.19	0.19
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 40 and name N)	7.25	0.20	0.20
80	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 41 and name CA)	8.62	0.18	0.18
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 41 and name CB)	8.34	0.25	0.24
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 42 and name CA)	6.97	0.23	0.23
	assign (segid 3A4 and resid 33 and name CB) (segid 3A4 and resid 42 and name CB)	5.61	0.26	0.25

	assign (segid 3A4 and resid 33 and name CB)	(segid 3A4 and resid 42 and name N)	7.05	0.19	0.20
	assign (segid 3A4 and resid 33 and name CB)	(segid 3A4 and resid 431 and name CA)	16.63	1.55	1.55
	assign (segid 3A4 and resid 33 and name N)	(segid 3A4 and resid 33 and name C)	2.39	0.03	0.03
	assign (segid 3A4 and resid 33 and name N)	(segid 3A4 and resid 33 and name CA)	1.45	0.00	0.01
5	assign (segid 3A4 and resid 33 and name N)	(segid 3A4 and resid 33 and name CB)	2.47	0.03	0.02
	assign (segid 3A4 and resid 33 and name N)	(segid 3A4 and resid 33 and name O)	2.81	0.08	0.08
	assign (segid 3A4 and resid 33 and name N)	(segid 3A4 and resid 343 and name C)	6.03	0.15	0.16
	assign (segid 3A4 and resid 33 and name N)	(segid 3A4 and resid 343 and name CA)	6.28	0.15	0.16
	assign (segid 3A4 and resid 33 and name N)	(segid 3A4 and resid 343 and name CB)	6.23	0.22	0.22
10	assign (segid 3A4 and resid 33 and name N)	(segid 3A4 and resid 343 and name N)	7.70	0.15	0.14
	assign (segid 3A4 and resid 33 and name N)	(segid 3A4 and resid 343 and name O)	6.94	0.22	0.21
	assign (segid 3A4 and resid 33 and name N)	(segid 3A4 and resid 344 and name C)	4.26	0.08	0.09
	assign (segid 3A4 and resid 33 and name N)	(segid 3A4 and resid 344 and name CA)	5.22	0.10	0.10
	assign (segid 3A4 and resid 33 and name N)	(segid 3A4 and resid 344 and name CB)	5.56	0.25	0.24
15	assign (segid 3A4 and resid 33 and name N)	(segid 3A4 and resid 344 and name N)	5.07	0.12	0.11
	assign (segid 3A4 and resid 33 and name N)	(segid 3A4 and resid 344 and name O)	3.08	0.07	0.07
	assign (segid 3A4 and resid 33 and name N)	(segid 3A4 and resid 345 and name C)	5.49	0.23	0.24
	assign (segid 3A4 and resid 33 and name N)	(segid 3A4 and resid 345 and name CA)	4.80	0.17	0.18
	assign (segid 3A4 and resid 33 and name N)	(segid 3A4 and resid 345 and name CB)	5.85	0.25	0.25
20	assign (segid 3A4 and resid 33 and name N)	(segid 3A4 and resid 345 and name N)	4.99	0.13	0.12
	assign (segid 3A4 and resid 33 and name N)	(segid 3A4 and resid 345 and name O)	6.66	0.23	0.24
	assign (segid 3A4 and resid 33 and name N)	(segid 3A4 and resid 346 and name C)	7.10	0.34	0.35
	assign (segid 3A4 and resid 33 and name N)	(segid 3A4 and resid 346 and name CA)	6.13	0.38	0.38
	assign (segid 3A4 and resid 33 and name N)	(segid 3A4 and resid 346 and name CB)	5.80	0.43	0.43
25	assign (segid 3A4 and resid 33 and name N)	(segid 3A4 and resid 346 and name N)	5.05	0.29	0.30
	assign (segid 3A4 and resid 33 and name N)	(segid 3A4 and resid 346 and name O)	7.14	0.29	0.29
	assign (segid 3A4 and resid 33 and name N)	(segid 3A4 and resid 34 and name C)	5.83	0.12	0.13
	assign (segid 3A4 and resid 33 and name N)	(segid 3A4 and resid 34 and name CA)	4.63	0.10	0.09
	assign (segid 3A4 and resid 33 and name N)	(segid 3A4 and resid 34 and name CB)	5.28	0.10	0.09
30	assign (segid 3A4 and resid 33 and name N)	(segid 3A4 and resid 34 and name N)	3.40	0.10	0.10
	assign (segid 3A4 and resid 33 and name N)	(segid 3A4 and resid 34 and name O)	6.83	0.12	0.12
	assign (segid 3A4 and resid 33 and name N)	(segid 3A4 and resid 35 and name CA)	7.44	0.20	0.20
	assign (segid 3A4 and resid 33 and name N)	(segid 3A4 and resid 35 and name N)	6.08	0.19	0.19
	assign (segid 3A4 and resid 33 and name N)	(segid 3A4 and resid 35 and name O)	7.09	0.15	0.14
35	assign (segid 3A4 and resid 33 and name N)	(segid 3A4 and resid 38 and name C)	7.20	0.27	0.28
	assign (segid 3A4 and resid 33 and name N)	(segid 3A4 and resid 38 and name CB)	6.54	0.28	0.27
	assign (segid 3A4 and resid 33 and name N)	(segid 3A4 and resid 39 and name CA)	7.11	0.21	0.22
	assign (segid 3A4 and resid 33 and name N)	(segid 3A4 and resid 39 and name CB)	7.14	0.18	0.17
	assign (segid 3A4 and resid 33 and name N)	(segid 3A4 and resid 39 and name N)	7.06	0.21	0.20
40	assign (segid 3A4 and resid 33 and name N)	(segid 3A4 and resid 42 and name CB)	7.59	0.20	0.20
	assign (segid 3A4 and resid 33 and name O)	(segid 3A4 and resid 33 and name CB)	3.02	0.11	0.11
	assign (segid 3A4 and resid 33 and name O)	(segid 3A4 and resid 343 and name C)	7.66	0.17	0.17
	assign (segid 3A4 and resid 33 and name O)	(segid 3A4 and resid 344 and name C)	4.88	0.14	0.13
	assign (segid 3A4 and resid 33 and name O)	(segid 3A4 and resid 344 and name CA)	6.23	0.11	0.12
45	assign (segid 3A4 and resid 33 and name O)	(segid 3A4 and resid 344 and name CB)	6.57	0.21	0.21
	assign (segid 3A4 and resid 33 and name O)	(segid 3A4 and resid 344 and name N)	6.65	0.15	0.16
	assign (segid 3A4 and resid 33 and name O)	(segid 3A4 and resid 344 and name O)	3.96	0.13	0.13
	assign (segid 3A4 and resid 33 and name O)	(segid 3A4 and resid 345 and name C)	4.20	0.38	0.37
50	assign (segid 3A4 and resid 33 and name O)	(segid 3A4 and resid 345 and name CA)	4.11	0.31	0.31
	assign (segid 3A4 and resid 33 and name O)	(segid 3A4 and resid 345 and name CB)	5.07	0.43	0.44
	assign (segid 3A4 and resid 33 and name O)	(segid 3A4 and resid 345 and name N)	4.97	0.19	0.20
	assign (segid 3A4 and resid 33 and name O)	(segid 3A4 and resid 345 and name O)	5.36	0.37	0.36
	assign (segid 3A4 and resid 33 and name O)	(segid 3A4 and resid 346 and name C)	4.74	0.50	0.50
55	assign (segid 3A4 and resid 33 and name O)	(segid 3A4 and resid 346 and name CA)	4.15	0.50	0.50
	assign (segid 3A4 and resid 33 and name O)	(segid 3A4 and resid 346 and name CB)	3.87	0.43	0.42
	assign (segid 3A4 and resid 33 and name O)	(segid 3A4 and resid 346 and name N)	3.32	0.44	0.45
	assign (segid 3A4 and resid 33 and name O)	(segid 3A4 and resid 346 and name O)	4.54	0.42	0.43
	assign (segid 3A4 and resid 33 and name O)	(segid 3A4 and resid 347 and name N)	5.90	0.55	0.54
60	assign (segid 3A4 and resid 33 and name O)	(segid 3A4 and resid 349 and name C)	6.77	0.42	0.42
	assign (segid 3A4 and resid 33 and name O)	(segid 3A4 and resid 349 and name CA)	6.56	0.27	0.27
	assign (segid 3A4 and resid 33 and name O)	(segid 3A4 and resid 349 and name CB)	5.38	0.20	0.20
	assign (segid 3A4 and resid 33 and name O)	(segid 3A4 and resid 349 and name N)	6.79	0.28	0.28
	assign (segid 3A4 and resid 33 and name O)	(segid 3A4 and resid 34 and name C)	3.81	0.10	0.11
	assign (segid 3A4 and resid 33 and name O)	(segid 3A4 and resid 34 and name CA)	2.80	0.02	0.03
65	assign (segid 3A4 and resid 33 and name O)	(segid 3A4 and resid 34 and name CB)	3.95	0.08	0.09
	assign (segid 3A4 and resid 33 and name O)	(segid 3A4 and resid 34 and name N)	2.27	0.02	0.01
	assign (segid 3A4 and resid 33 and name O)	(segid 3A4 and resid 34 and name O)	4.54	0.15	0.15
	assign (segid 3A4 and resid 33 and name O)	(segid 3A4 and resid 350 and name N)	6.43	0.65	0.66
	assign (segid 3A4 and resid 33 and name O)	(segid 3A4 and resid 35 and name C)	5.85	0.23	0.23
70	assign (segid 3A4 and resid 33 and name O)	(segid 3A4 and resid 35 and name CA)	5.69	0.21	0.20
	assign (segid 3A4 and resid 33 and name O)	(segid 3A4 and resid 35 and name N)	4.41	0.20	0.19
	assign (segid 3A4 and resid 33 and name O)	(segid 3A4 and resid 35 and name O)	5.28	0.27	0.27
	assign (segid 3A4 and resid 33 and name O)	(segid 3A4 and resid 36 and name N)	6.95	0.24	0.25
	assign (segid 3A4 and resid 33 and name O)	(segid 3A4 and resid 38 and name C)	6.58	0.41	0.40
75	assign (segid 3A4 and resid 33 and name O)	(segid 3A4 and resid 38 and name CA)	7.07	0.37	0.38
	assign (segid 3A4 and resid 33 and name O)	(segid 3A4 and resid 38 and name CB)	6.29	0.39	0.39
	assign (segid 3A4 and resid 33 and name O)	(segid 3A4 and resid 39 and name CA)	5.87	0.40	0.40
	assign (segid 3A4 and resid 33 and name O)	(segid 3A4 and resid 39 and name CB)	5.35	0.34	0.34
	assign (segid 3A4 and resid 33 and name O)	(segid 3A4 and resid 39 and name N)	5.94	0.37	0.37
80	assign (segid 3A4 and resid 33 and name O)	(segid 3A4 and resid 340 and name O)	1.24	0.01	0.01
	assign (segid 3A4 and resid 340 and name C)	(segid 3A4 and resid 341 and name C)	3.10	0.10	0.11
	assign (segid 3A4 and resid 340 and name C)	(segid 3A4 and resid 341 and name CA)	2.43	0.01	0.02
	assign (segid 3A4 and resid 340 and name C)	(segid 3A4 and resid 341 and name CB)	3.69	0.03	0.04

	assign (segid 3A4 and resid 340 and name C) (segid 3A4 and resid 341 and name CG)	4.18	0.17	0.16
	assign (segid 3A4 and resid 340 and name C) (segid 3A4 and resid 341 and name N)	1.33	0.00	0.01
	assign (segid 3A4 and resid 340 and name C) (segid 3A4 and resid 341 and name O)	3.38	0.11	0.11
	assign (segid 3A4 and resid 340 and name C) (segid 3A4 and resid 342 and name C)	6.29	0.12	0.12
	assign (segid 3A4 and resid 340 and name C) (segid 3A4 and resid 342 and name CA)	5.16	0.15	0.15
5	assign (segid 3A4 and resid 340 and name C) (segid 3A4 and resid 342 and name N)	4.02	0.13	0.13
	assign (segid 3A4 and resid 340 and name C) (segid 3A4 and resid 342 and name O)	6.68	0.13	0.13
	assign (segid 3A4 and resid 340 and name C) (segid 3A4 and resid 343 and name N)	7.06	0.16	0.17
	assign (segid 3A4 and resid 340 and name C) (segid 3A4 and resid 340 and name C)	1.52	0.00	0.01
	assign (segid 3A4 and resid 340 and name CA) (segid 3A4 and resid 340 and name O)	2.39	0.02	0.01
10	assign (segid 3A4 and resid 340 and name CA) (segid 3A4 and resid 341 and name C)	4.44	0.09	0.08
	assign (segid 3A4 and resid 340 and name CA) (segid 3A4 and resid 341 and name CA)	3.82	0.01	0.01
	assign (segid 3A4 and resid 340 and name CA) (segid 3A4 and resid 341 and name CB)	4.88	0.04	0.03
	assign (segid 3A4 and resid 340 and name CA) (segid 3A4 and resid 341 and name CG)	5.20	0.19	0.19
	assign (segid 3A4 and resid 340 and name CA) (segid 3A4 and resid 341 and name N)	2.44	0.01	0.02
15	assign (segid 3A4 and resid 340 and name CA) (segid 3A4 and resid 341 and name O)	4.42	0.11	0.10
	assign (segid 3A4 and resid 340 and name CA) (segid 3A4 and resid 342 and name C)	7.61	0.09	0.09
	assign (segid 3A4 and resid 340 and name CA) (segid 3A4 and resid 342 and name CA)	6.48	0.13	0.14
	assign (segid 3A4 and resid 340 and name CA) (segid 3A4 and resid 342 and name N)	5.45	0.11	0.11
	assign (segid 3A4 and resid 340 and name CA) (segid 3A4 and resid 343 and name CA)	9.48	0.14	0.15
20	assign (segid 3A4 and resid 340 and name CA) (segid 3A4 and resid 343 and name CB)	9.53	0.17	0.16
	assign (segid 3A4 and resid 340 and name CA) (segid 3A4 and resid 344 and name CA)	12.95	0.19	0.18
	assign (segid 3A4 and resid 340 and name CA) (segid 3A4 and resid 344 and name CB)	13.57	0.26	0.25
	assign (segid 3A4 and resid 340 and name CA) (segid 3A4 and resid 345 and name CA)	15.61	0.17	0.16
	assign (segid 3A4 and resid 340 and name CA) (segid 3A4 and resid 345 and name CB)	15.59	0.34	0.33
25	assign (segid 3A4 and resid 340 and name CA) (segid 3A4 and resid 346 and name CA)	18.95	0.23	0.23
	assign (segid 3A4 and resid 340 and name CA) (segid 3A4 and resid 346 and name CB)	19.39	0.28	0.28
	assign (segid 3A4 and resid 340 and name CA) (segid 3A4 and resid 389 and name CB)	17.82	1.46	1.46
	assign (segid 3A4 and resid 340 and name N) (segid 3A4 and resid 340 and name C)	2.51	0.01	0.02
	assign (segid 3A4 and resid 340 and name N) (segid 3A4 and resid 340 and name CA)	1.46	0.01	0.00
30	assign (segid 3A4 and resid 340 and name N) (segid 3A4 and resid 340 and name O)	3.64	0.02	0.01
	assign (segid 3A4 and resid 340 and name N) (segid 3A4 and resid 341 and name C)	4.94	0.12	0.11
	assign (segid 3A4 and resid 340 and name N) (segid 3A4 and resid 341 and name CA)	4.23	0.04	0.03
	assign (segid 3A4 and resid 340 and name N) (segid 3A4 and resid 341 and name CB)	4.91	0.05	0.04
	assign (segid 3A4 and resid 340 and name N) (segid 3A4 and resid 341 and name CG)	5.13	0.22	0.22
35	assign (segid 3A4 and resid 340 and name N) (segid 3A4 and resid 341 and name N)	2.78	0.05	0.04
	assign (segid 3A4 and resid 340 and name N) (segid 3A4 and resid 341 and name O)	4.73	0.13	0.14
	assign (segid 3A4 and resid 340 and name N) (segid 3A4 and resid 342 and name CA)	7.17	0.14	0.14
	assign (segid 3A4 and resid 340 and name N) (segid 3A4 and resid 342 and name N)	6.13	0.12	0.11
	assign (segid 3A4 and resid 340 and name N) (segid 3A4 and resid 341 and name C)	3.19	0.18	0.19
40	assign (segid 3A4 and resid 340 and name O) (segid 3A4 and resid 341 and name CA)	2.77	0.03	0.02
	assign (segid 3A4 and resid 340 and name O) (segid 3A4 and resid 341 and name CB)	4.20	0.06	0.07
	assign (segid 3A4 and resid 340 and name O) (segid 3A4 and resid 341 and name CG)	4.72	0.22	0.22
	assign (segid 3A4 and resid 340 and name O) (segid 3A4 and resid 341 and name N)	2.26	0.02	0.02
	assign (segid 3A4 and resid 340 and name O) (segid 3A4 and resid 341 and name O)	3.68	0.21	0.22
45	assign (segid 3A4 and resid 340 and name O) (segid 3A4 and resid 342 and name C)	6.09	0.26	0.26
	assign (segid 3A4 and resid 340 and name O) (segid 3A4 and resid 342 and name CA)	4.79	0.29	0.30
	assign (segid 3A4 and resid 340 and name O) (segid 3A4 and resid 342 and name N)	3.73	0.23	0.24
	assign (segid 3A4 and resid 340 and name O) (segid 3A4 and resid 343 and name N)	6.50	0.22	0.22
	assign (segid 3A4 and resid 340 and name O) (segid 3A4 and resid 343 and name CA)	6.94	0.30	0.30
50	assign (segid 3A4 and resid 341 and name C) (segid 3A4 and resid 341 and name CB)	2.48	0.04	0.03
	assign (segid 3A4 and resid 341 and name C) (segid 3A4 and resid 341 and name CG)	3.81	0.06	0.06
	assign (segid 3A4 and resid 341 and name C) (segid 3A4 and resid 341 and name O)	1.23	0.01	0.01
	assign (segid 3A4 and resid 341 and name C) (segid 3A4 and resid 342 and name C)	3.26	0.04	0.04
	assign (segid 3A4 and resid 341 and name C) (segid 3A4 and resid 342 and name CA)	2.44	0.02	0.01
55	assign (segid 3A4 and resid 341 and name C) (segid 3A4 and resid 342 and name N)	1.33	0.01	0.01
	assign (segid 3A4 and resid 341 and name C) (segid 3A4 and resid 342 and name O)	3.65	0.06	0.07
	assign (segid 3A4 and resid 341 and name C) (segid 3A4 and resid 343 and name C)	6.50	0.11	0.11
	assign (segid 3A4 and resid 341 and name C) (segid 3A4 and resid 343 and name CA)	5.28	0.11	0.11
	assign (segid 3A4 and resid 341 and name C) (segid 3A4 and resid 343 and name CB)	5.62	0.12	0.13
60	assign (segid 3A4 and resid 341 and name C) (segid 3A4 and resid 343 and name N)	4.09	0.10	0.11
	assign (segid 3A4 and resid 341 and name C) (segid 3A4 and resid 343 and name O)	6.75	0.14	0.15
	assign (segid 3A4 and resid 341 and name C) (segid 3A4 and resid 344 and name N)	7.49	0.12	0.12
	assign (segid 3A4 and resid 341 and name C) (segid 3A4 and resid 341 and name C)	1.52	0.01	0.02
	assign (segid 3A4 and resid 341 and name CA) (segid 3A4 and resid 341 and name CB)	1.52	0.01	0.02
65	assign (segid 3A4 and resid 341 and name CA) (segid 3A4 and resid 341 and name CG)	2.52	0.05	0.05
	assign (segid 3A4 and resid 341 and name CA) (segid 3A4 and resid 341 and name O)	2.39	0.01	0.02
	assign (segid 3A4 and resid 341 and name CA) (segid 3A4 and resid 342 and name C)	4.52	0.06	0.06
	assign (segid 3A4 and resid 341 and name CA) (segid 3A4 and resid 342 and name CA)	3.79	0.02	0.02
	assign (segid 3A4 and resid 341 and name CA) (segid 3A4 and resid 342 and name N)	2.41	0.02	0.02
70	assign (segid 3A4 and resid 341 and name CA) (segid 3A4 and resid 342 and name O)	4.61	0.12	0.11
	assign (segid 3A4 and resid 341 and name CA) (segid 3A4 and resid 343 and name CA)	6.53	0.15	0.16
	assign (segid 3A4 and resid 341 and name CA) (segid 3A4 and resid 343 and name CB)	6.80	0.20	0.20
	assign (segid 3A4 and resid 341 and name CA) (segid 3A4 and resid 343 and name N)	5.46	0.12	0.13
	assign (segid 3A4 and resid 341 and name CA) (segid 3A4 and resid 344 and name CA)	10.08	0.16	0.16
75	assign (segid 3A4 and resid 341 and name CA) (segid 3A4 and resid 344 and name CB)	10.56	0.19	0.19
	assign (segid 3A4 and resid 341 and name CA) (segid 3A4 and resid 345 and name CA)	12.93	0.22	0.23
	assign (segid 3A4 and resid 341 and name CA) (segid 3A4 and resid 345 and name CB)	13.18	0.34	0.34
	assign (segid 3A4 and resid 341 and name CA) (segid 3A4 and resid 346 and name CA)	16.05	0.26	0.25
	assign (segid 3A4 and resid 341 and name CA) (segid 3A4 and resid 346 and name CB)	16.29	0.30	0.30
80	assign (segid 3A4 and resid 341 and name CA) (segid 3A4 and resid 347 and name CA)	18.86	0.28	0.28
	assign (segid 3A4 and resid 341 and name CA) (segid 3A4 and resid 347 and name CB)	19.24	0.30	0.30
	assign (segid 3A4 and resid 341 and name CA) (segid 3A4 and resid 349 and name CB)	19.42	0.27	0.28

	assign (segid 3A4 and resid 341 and name CA)	(segid 3A4 and resid 389 and name CB)	17.65	1.17	1.17
	assign (segid 3A4 and resid 341 and name CB)	(segid 3A4 and resid 341 and name CG)	1.49	0.04	0.03
	assign (segid 3A4 and resid 341 and name CB)	(segid 3A4 and resid 342 and name C)	4.77	0.13	0.13
	assign (segid 3A4 and resid 341 and name CB)	(segid 3A4 and resid 342 and name CA)	4.51	0.05	0.06
5	assign (segid 3A4 and resid 341 and name CB)	(segid 3A4 and resid 342 and name N)	3.23	0.05	0.05
	assign (segid 3A4 and resid 341 and name CB)	(segid 3A4 and resid 342 and name O)	4.55	0.15	0.16
	assign (segid 3A4 and resid 341 and name CB)	(segid 3A4 and resid 343 and name CA)	6.46	0.26	0.27
	assign (segid 3A4 and resid 341 and name CB)	(segid 3A4 and resid 343 and name CB)	6.57	0.33	0.34
	assign (segid 3A4 and resid 341 and name CB)	(segid 3A4 and resid 343 and name N)	5.68	0.22	0.21
	assign (segid 3A4 and resid 341 and name CB)	(segid 3A4 and resid 344 and name CA)	10.10	0.28	0.28
10	assign (segid 3A4 and resid 341 and name CB)	(segid 3A4 and resid 344 and name CB)	10.60	0.28	0.28
	assign (segid 3A4 and resid 341 and name CB)	(segid 3A4 and resid 345 and name CA)	12.76	0.36	0.35
	assign (segid 3A4 and resid 341 and name CB)	(segid 3A4 and resid 345 and name CB)	13.04	0.43	0.43
	assign (segid 3A4 and resid 341 and name CB)	(segid 3A4 and resid 346 and name CA)	15.83	0.37	0.38
	assign (segid 3A4 and resid 341 and name CB)	(segid 3A4 and resid 346 and name CB)	16.00	0.40	0.39
15	assign (segid 3A4 and resid 341 and name CB)	(segid 3A4 and resid 347 and name CA)	18.72	0.40	0.39
	assign (segid 3A4 and resid 341 and name CB)	(segid 3A4 and resid 347 and name CB)	19.20	0.40	0.40
	assign (segid 3A4 and resid 341 and name CB)	(segid 3A4 and resid 349 and name CB)	18.93	0.38	0.37
	assign (segid 3A4 and resid 341 and name CB)	(segid 3A4 and resid 389 and name CB)	18.19	1.12	1.12
	assign (segid 3A4 and resid 341 and name CG)	(segid 3A4 and resid 342 and name C)	6.08	0.15	0.15
20	assign (segid 3A4 and resid 341 and name CG)	(segid 3A4 and resid 342 and name CA)	5.82	0.06	0.06
	assign (segid 3A4 and resid 341 and name CG)	(segid 3A4 and resid 342 and name N)	4.46	0.05	0.06
	assign (segid 3A4 and resid 341 and name CG)	(segid 3A4 and resid 342 and name O)	5.71	0.22	0.22
	assign (segid 3A4 and resid 341 and name CG)	(segid 3A4 and resid 343 and name N)	7.04	0.23	0.23
	assign (segid 3A4 and resid 341 and name N)	(segid 3A4 and resid 341 and name C)	2.44	0.02	0.01
25	assign (segid 3A4 and resid 341 and name N)	(segid 3A4 and resid 341 and name CA)	1.46	0.01	0.02
	assign (segid 3A4 and resid 341 and name N)	(segid 3A4 and resid 341 and name CB)	2.47	0.03	0.02
	assign (segid 3A4 and resid 341 and name N)	(segid 3A4 and resid 341 and name CG)	3.07	0.14	0.15
	assign (segid 3A4 and resid 341 and name N)	(segid 3A4 and resid 341 and name O)	2.76	0.05	0.04
	assign (segid 3A4 and resid 341 and name N)	(segid 3A4 and resid 342 and name C)	5.68	0.04	0.03
30	assign (segid 3A4 and resid 341 and name N)	(segid 3A4 and resid 342 and name CA)	1.80	0.03	0.03
	assign (segid 3A4 and resid 341 and name N)	(segid 3A4 and resid 342 and name N)	3.55	0.03	0.03
	assign (segid 3A4 and resid 341 and name N)	(segid 3A4 and resid 342 and name O)	5.93	0.09	0.09
	assign (segid 3A4 and resid 341 and name N)	(segid 3A4 and resid 343 and name CA)	7.57	0.16	0.16
	assign (segid 3A4 and resid 341 and name N)	(segid 3A4 and resid 343 and name N)	6.46	0.13	0.13
35	assign (segid 3A4 and resid 341 and name O)	(segid 3A4 and resid 341 and name CB)	3.15	0.09	0.08
	assign (segid 3A4 and resid 341 and name O)	(segid 3A4 and resid 341 and name CG)	4.53	0.10	0.09
	assign (segid 3A4 and resid 341 and name O)	(segid 3A4 and resid 342 and name C)	3.50	0.08	0.09
	assign (segid 3A4 and resid 341 and name O)	(segid 3A4 and resid 342 and name CA)	2.80	0.03	0.04
40	assign (segid 3A4 and resid 341 and name O)	(segid 3A4 and resid 342 and name N)	2.27	0.02	0.01
	assign (segid 3A4 and resid 341 and name O)	(segid 3A4 and resid 342 and name O)	4.13	0.12	0.13
	assign (segid 3A4 and resid 341 and name O)	(segid 3A4 and resid 343 and name C)	6.31	0.13	0.12
	assign (segid 3A4 and resid 341 and name O)	(segid 3A4 and resid 343 and name CA)	5.12	0.15	0.14
	assign (segid 3A4 and resid 341 and name O)	(segid 3A4 and resid 343 and name CB)	5.20	0.16	0.16
	assign (segid 3A4 and resid 341 and name O)	(segid 3A4 and resid 343 and name N)	3.96	0.13	0.14
45	assign (segid 3A4 and resid 341 and name O)	(segid 3A4 and resid 343 and name O)	6.42	0.15	0.15
	assign (segid 3A4 and resid 341 and name O)	(segid 3A4 and resid 344 and name N)	7.42	0.13	0.13
	assign (segid 3A4 and resid 342 and name C)	(segid 3A4 and resid 342 and name O)	1.23	0.00	0.00
	assign (segid 3A4 and resid 342 and name C)	(segid 3A4 and resid 343 and name C)	3.48	0.06	0.07
50	assign (segid 3A4 and resid 342 and name C)	(segid 3A4 and resid 343 and name CA)	2.44	0.02	0.01
	assign (segid 3A4 and resid 342 and name C)	(segid 3A4 and resid 343 and name CB)	3.48	0.08	0.08
	assign (segid 3A4 and resid 342 and name C)	(segid 3A4 and resid 343 and name N)	1.32	0.02	0.02
	assign (segid 3A4 and resid 342 and name C)	(segid 3A4 and resid 343 and name O)	3.97	0.11	0.11
	assign (segid 3A4 and resid 342 and name C)	(segid 3A4 and resid 344 and name C)	6.67	0.07	0.08
	assign (segid 3A4 and resid 342 and name C)	(segid 3A4 and resid 344 and name CA)	5.60	0.10	0.10
55	assign (segid 3A4 and resid 342 and name C)	(segid 3A4 and resid 344 and name CB)	6.08	0.17	0.17
	assign (segid 3A4 and resid 342 and name C)	(segid 3A4 and resid 344 and name N)	4.33	0.08	0.07
	assign (segid 3A4 and resid 342 and name C)	(segid 3A4 and resid 344 and name O)	6.96	0.11	0.11
	assign (segid 3A4 and resid 342 and name C)	(segid 3A4 and resid 345 and name N)	7.54	0.12	0.11
	assign (segid 3A4 and resid 342 and name C)	(segid 3A4 and resid 342 and name O)	1.53	0.01	0.01
60	assign (segid 3A4 and resid 342 and name CA)	(segid 3A4 and resid 342 and name C)	2.41	0.02	0.01
	assign (segid 3A4 and resid 342 and name CA)	(segid 3A4 and resid 343 and name C)	4.67	0.09	0.08
	assign (segid 3A4 and resid 342 and name CA)	(segid 3A4 and resid 343 and name CA)	3.80	0.02	0.02
	assign (segid 3A4 and resid 342 and name CA)	(segid 3A4 and resid 343 and name CB)	4.70	0.05	0.04
	assign (segid 3A4 and resid 342 and name CA)	(segid 3A4 and resid 343 and name N)	2.42	0.03	0.02
65	assign (segid 3A4 and resid 342 and name CA)	(segid 3A4 and resid 343 and name O)	4.85	0.14	0.15
	assign (segid 3A4 and resid 342 and name CA)	(segid 3A4 and resid 344 and name CA)	6.75	0.10	0.11
	assign (segid 3A4 and resid 342 and name CA)	(segid 3A4 and resid 344 and name CB)	7.18	0.20	0.20
	assign (segid 3A4 and resid 342 and name CA)	(segid 3A4 and resid 344 and name N)	5.61	0.08	0.08
	assign (segid 3A4 and resid 342 and name CA)	(segid 3A4 and resid 345 and name CA)	9.96	0.13	0.14
70	assign (segid 3A4 and resid 342 and name CA)	(segid 3A4 and resid 345 and name CB)	10.31	0.31	0.32
	assign (segid 3A4 and resid 342 and name CA)	(segid 3A4 and resid 346 and name CA)	12.92	0.22	0.23
	assign (segid 3A4 and resid 342 and name CA)	(segid 3A4 and resid 346 and name CB)	13.27	0.29	0.29
	assign (segid 3A4 and resid 342 and name CA)	(segid 3A4 and resid 347 and name CB)	15.99	0.28	0.29
	assign (segid 3A4 and resid 342 and name CA)	(segid 3A4 and resid 348 and name CA)	18.17	0.28	0.28
75	assign (segid 3A4 and resid 342 and name CA)	(segid 3A4 and resid 349 and name CA)	17.81	0.20	0.20
	assign (segid 3A4 and resid 342 and name CA)	(segid 3A4 and resid 349 and name CB)	16.72	0.21	0.20
	assign (segid 3A4 and resid 342 and name CA)	(segid 3A4 and resid 350 and name CA)	18.37	0.53	0.53
	assign (segid 3A4 and resid 342 and name CA)	(segid 3A4 and resid 350 and name CB)	17.72	0.66	0.66
80	assign (segid 3A4 and resid 342 and name CA)	(segid 3A4 and resid 382 and name CB)	18.30	0.63	0.63
	assign (segid 3A4 and resid 342 and name CA)	(segid 3A4 and resid 385 and name CA)	17.13	0.72	0.71
	assign (segid 3A4 and resid 342 and name CA)	(segid 3A4 and resid 386 and name CA)	17.51	0.87	0.87

	assign (segid 3A4 and resid 342 and name CA)	(segid 3A4 and resid 387 and name CA)	17.52	1.00	1.01
	assign (segid 3A4 and resid 342 and name CA)	(segid 3A4 and resid 388 and name CA)	18.20	0.84	0.85
	assign (segid 3A4 and resid 342 and name CA)	(segid 3A4 and resid 388 and name CB)	17.92	0.85	0.86
	assign (segid 3A4 and resid 342 and name CA)	(segid 3A4 and resid 389 and name CA)	16.69	0.98	0.98
	assign (segid 3A4 and resid 342 and name CA)	(segid 3A4 and resid 389 and name CB)	15.25	1.00	1.00
5	assign (segid 3A4 and resid 342 and name CA)	(segid 3A4 and resid 342 and name C)	2.44	0.05	0.05
	assign (segid 3A4 and resid 342 and name N)	(segid 3A4 and resid 342 and name C)	1.46	0.02	0.01
	assign (segid 3A4 and resid 342 and name N)	(segid 3A4 and resid 342 and name O)	2.81	0.08	0.07
	assign (segid 3A4 and resid 342 and name N)	(segid 3A4 and resid 343 and name C)	5.87	0.11	0.10
	assign (segid 3A4 and resid 342 and name N)	(segid 3A4 and resid 343 and name CA)	4.77	0.08	0.09
10	assign (segid 3A4 and resid 342 and name N)	(segid 3A4 and resid 343 and name CB)	5.47	0.09	0.10
	assign (segid 3A4 and resid 342 and name N)	(segid 3A4 and resid 343 and name N)	3.52	0.07	0.08
	assign (segid 3A4 and resid 342 and name N)	(segid 3A4 and resid 343 and name O)	6.17	0.15	0.15
	assign (segid 3A4 and resid 342 and name N)	(segid 3A4 and resid 344 and name N)	6.76	0.12	0.12
	assign (segid 3A4 and resid 342 and name N)	(segid 3A4 and resid 343 and name C)	3.92	0.10	0.10
15	assign (segid 3A4 and resid 342 and name O)	(segid 3A4 and resid 343 and name CA)	2.78	0.04	0.04
	assign (segid 3A4 and resid 342 and name O)	(segid 3A4 and resid 343 and name CB)	3.82	0.15	0.14
	assign (segid 3A4 and resid 342 and name O)	(segid 3A4 and resid 343 and name N)	2.24	0.02	0.02
	assign (segid 3A4 and resid 342 and name O)	(segid 3A4 and resid 343 and name O)	4.68	0.13	0.13
20	assign (segid 3A4 and resid 342 and name O)	(segid 3A4 and resid 344 and name C)	6.79	0.13	0.13
	assign (segid 3A4 and resid 342 and name O)	(segid 3A4 and resid 344 and name CA)	5.79	0.16	0.16
	assign (segid 3A4 and resid 342 and name O)	(segid 3A4 and resid 344 and name CB)	6.11	0.24	0.23
	assign (segid 3A4 and resid 342 and name O)	(segid 3A4 and resid 344 and name N)	4.46	0.13	0.12
	assign (segid 3A4 and resid 342 and name O)	(segid 3A4 and resid 344 and name O)	6.87	0.14	0.15
25	assign (segid 3A4 and resid 342 and name O)	(segid 3A4 and resid 345 and name N)	7.80	0.16	0.15
	assign (segid 3A4 and resid 342 and name O)	(segid 3A4 and resid 343 and name CB)	2.50	0.06	0.05
	assign (segid 3A4 and resid 343 and name C)	(segid 3A4 and resid 343 and name O)	1.23	0.01	0.00
	assign (segid 3A4 and resid 343 and name C)	(segid 3A4 and resid 344 and name C)	3.36	0.10	0.10
	assign (segid 3A4 and resid 343 and name C)	(segid 3A4 and resid 344 and name CA)	2.43	0.02	0.02
	assign (segid 3A4 and resid 343 and name C)	(segid 3A4 and resid 344 and name CB)	3.50	0.08	0.08
30	assign (segid 3A4 and resid 343 and name C)	(segid 3A4 and resid 344 and name N)	1.33	0.00	0.00
	assign (segid 3A4 and resid 343 and name C)	(segid 3A4 and resid 344 and name O)	3.92	0.16	0.15
	assign (segid 3A4 and resid 343 and name C)	(segid 3A4 and resid 345 and name C)	6.47	0.13	0.13
	assign (segid 3A4 and resid 343 and name C)	(segid 3A4 and resid 345 and name CA)	5.33	0.13	0.13
	assign (segid 3A4 and resid 343 and name C)	(segid 3A4 and resid 345 and name CB)	5.82	0.26	0.26
35	assign (segid 3A4 and resid 343 and name C)	(segid 3A4 and resid 345 and name N)	4.09	0.12	0.11
	assign (segid 3A4 and resid 343 and name C)	(segid 3A4 and resid 345 and name O)	6.95	0.14	0.14
	assign (segid 3A4 and resid 343 and name C)	(segid 3A4 and resid 346 and name N)	7.17	0.19	0.18
	assign (segid 3A4 and resid 343 and name C)	(segid 3A4 and resid 343 and name C)	1.52	0.01	0.02
	assign (segid 3A4 and resid 343 and name CA)	(segid 3A4 and resid 343 and name CB)	1.55	0.01	0.00
40	assign (segid 3A4 and resid 343 and name CA)	(segid 3A4 and resid 343 and name O)	2.39	0.02	0.02
	assign (segid 3A4 and resid 343 and name CA)	(segid 3A4 and resid 344 and name C)	4.57	0.08	0.07
	assign (segid 3A4 and resid 343 and name CA)	(segid 3A4 and resid 344 and name CA)	3.79	0.03	0.03
	assign (segid 3A4 and resid 343 and name CA)	(segid 3A4 and resid 344 and name CB)	4.70	0.06	0.06
	assign (segid 3A4 and resid 343 and name CA)	(segid 3A4 and resid 344 and name N)	2.42	0.02	0.03
45	assign (segid 3A4 and resid 343 and name CA)	(segid 3A4 and resid 344 and name O)	4.83	0.15	0.16
	assign (segid 3A4 and resid 343 and name CA)	(segid 3A4 and resid 345 and name C)	7.70	0.12	0.11
	assign (segid 3A4 and resid 343 and name CA)	(segid 3A4 and resid 345 and name CA)	6.45	0.11	0.10
	assign (segid 3A4 and resid 343 and name CA)	(segid 3A4 and resid 345 and name CB)	6.86	0.26	0.27
	assign (segid 3A4 and resid 343 and name CA)	(segid 3A4 and resid 345 and name N)	5.36	0.10	0.10
50	assign (segid 3A4 and resid 343 and name CA)	(segid 3A4 and resid 346 and name C)	9.58	0.17	0.17
	assign (segid 3A4 and resid 343 and name CA)	(segid 3A4 and resid 346 and name CB)	9.95	0.27	0.27
	assign (segid 3A4 and resid 343 and name CA)	(segid 3A4 and resid 347 and name CA)	12.37	0.17	0.16
	assign (segid 3A4 and resid 343 and name CA)	(segid 3A4 and resid 347 and name CB)	12.81	0.21	0.21
	assign (segid 3A4 and resid 343 and name CA)	(segid 3A4 and resid 348 and name CA)	14.90	0.21	0.21
55	assign (segid 3A4 and resid 343 and name CA)	(segid 3A4 and resid 349 and name CA)	14.30	0.23	0.23
	assign (segid 3A4 and resid 343 and name CA)	(segid 3A4 and resid 349 and name CB)	13.21	0.23	0.24
	assign (segid 3A4 and resid 343 and name CA)	(segid 3A4 and resid 350 and name CA)	14.66	0.56	0.55
	assign (segid 3A4 and resid 343 and name CA)	(segid 3A4 and resid 350 and name CB)	14.02	0.69	0.69
	assign (segid 3A4 and resid 343 and name CA)	(segid 3A4 and resid 351 and name CA)	17.84	0.40	0.39
60	assign (segid 3A4 and resid 343 and name CA)	(segid 3A4 and resid 352 and name CA)	19.12	0.33	0.34
	assign (segid 3A4 and resid 343 and name CA)	(segid 3A4 and resid 352 and name CB)	18.95	0.39	0.40
	assign (segid 3A4 and resid 343 and name CA)	(segid 3A4 and resid 353 and name CB)	17.80	0.71	0.72
	assign (segid 3A4 and resid 343 and name CA)	(segid 3A4 and resid 382 and name CA)	16.24	0.47	0.47
	assign (segid 3A4 and resid 343 and name CA)	(segid 3A4 and resid 382 and name CB)	14.92	0.53	0.53
65	assign (segid 3A4 and resid 343 and name CA)	(segid 3A4 and resid 383 and name CA)	17.33	0.38	0.38
	assign (segid 3A4 and resid 343 and name CA)	(segid 3A4 and resid 384 and name CA)	17.60	0.52	0.52
	assign (segid 3A4 and resid 343 and name CA)	(segid 3A4 and resid 384 and name CB)	18.93	0.57	0.56
	assign (segid 3A4 and resid 343 and name CA)	(segid 3A4 and resid 385 and name CA)	14.39	0.62	0.61
	assign (segid 3A4 and resid 343 and name CA)	(segid 3A4 and resid 386 and name CA)	14.76	0.66	0.66
70	assign (segid 3A4 and resid 343 and name CA)	(segid 3A4 and resid 387 and name CA)	15.24	1.08	1.08
	assign (segid 3A4 and resid 343 and name CA)	(segid 3A4 and resid 388 and name CA)	16.59	0.93	0.94
	assign (segid 3A4 and resid 343 and name CA)	(segid 3A4 and resid 388 and name CB)	16.56	1.01	1.02
	assign (segid 3A4 and resid 343 and name CA)	(segid 3A4 and resid 389 and name CA)	15.17	0.95	0.95
	assign (segid 3A4 and resid 343 and name CA)	(segid 3A4 and resid 389 and name CB)	13.84	0.99	0.98
75	assign (segid 3A4 and resid 343 and name CA)	(segid 3A4 and resid 390 and name CA)	16.77	0.97	0.97
	assign (segid 3A4 and resid 343 and name CA)	(segid 3A4 and resid 390 and name CB)	17.64	0.97	0.96
	assign (segid 3A4 and resid 343 and name CA)	(segid 3A4 and resid 391 and name CA)	18.79	0.78	0.77
	assign (segid 3A4 and resid 343 and name CA)	(segid 3A4 and resid 391 and name CB)	19.10	0.62	0.62
	assign (segid 3A4 and resid 343 and name CA)	(segid 3A4 and resid 431 and name CA)	15.25	1.72	1.72
80	assign (segid 3A4 and resid 343 and name CA)	(segid 3A4 and resid 344 and name C)	4.96	0.08	0.09
	assign (segid 3A4 and resid 343 and name CB)	(segid 3A4 and resid 344 and name CA)	4.60	0.10	0.09
	assign (segid 3A4 and resid 343 and name CB)	(segid 3A4 and resid 344 and name CB)	5.75	0.10	0.10

	assign (segid 3A4 and resid 343 and name CB)	(segid 3A4 and resid 344 and name N)	3.35	0.08	0.07
	assign (segid 3A4 and resid 343 and name CB)	(segid 3A4 and resid 344 and name O)	5.14	0.20	0.21
	assign (segid 3A4 and resid 343 and name CB)	(segid 3A4 and resid 345 and name CA)	6.37	0.12	0.12
	assign (segid 3A4 and resid 343 and name CB)	(segid 3A4 and resid 345 and name CB)	6.52	0.25	0.26
	assign (segid 3A4 and resid 343 and name CB)	(segid 3A4 and resid 345 and name N)	5.53	0.13	0.12
5	assign (segid 3A4 and resid 343 and name CB)	(segid 3A4 and resid 346 and name CA)	9.79	0.17	0.17
	assign (segid 3A4 and resid 343 and name CB)	(segid 3A4 and resid 346 and name CB)	10.25	0.28	0.28
	assign (segid 3A4 and resid 343 and name CB)	(segid 3A4 and resid 347 and name CA)	12.30	0.19	0.20
	assign (segid 3A4 and resid 343 and name CB)	(segid 3A4 and resid 347 and name CB)	12.76	0.26	0.25
	assign (segid 3A4 and resid 343 and name CB)	(segid 3A4 and resid 348 and name CA)	15.06	0.16	0.17
10	assign (segid 3A4 and resid 343 and name CB)	(segid 3A4 and resid 349 and name CA)	14.33	0.25	0.24
	assign (segid 3A4 and resid 343 and name CB)	(segid 3A4 and resid 349 and name CB)	13.27	0.23	0.24
	assign (segid 3A4 and resid 343 and name CB)	(segid 3A4 and resid 350 and name CA)	14.30	0.61	0.62
	assign (segid 3A4 and resid 343 and name CB)	(segid 3A4 and resid 350 and name CB)	13.59	0.74	0.73
	assign (segid 3A4 and resid 343 and name CB)	(segid 3A4 and resid 351 and name CA)	17.57	0.47	0.47
15	assign (segid 3A4 and resid 343 and name CB)	(segid 3A4 and resid 352 and name CA)	18.98	0.42	0.42
	assign (segid 3A4 and resid 343 and name CB)	(segid 3A4 and resid 352 and name CB)	18.93	0.46	0.46
	assign (segid 3A4 and resid 343 and name CB)	(segid 3A4 and resid 353 and name CA)	18.27	0.68	0.67
	assign (segid 3A4 and resid 343 and name CB)	(segid 3A4 and resid 353 and name CB)	17.34	0.80	0.79
	assign (segid 3A4 and resid 343 and name CB)	(segid 3A4 and resid 381 and name CA)	18.75	0.79	0.79
20	assign (segid 3A4 and resid 343 and name CB)	(segid 3A4 and resid 382 and name CA)	15.74	0.56	0.57
	assign (segid 3A4 and resid 343 and name CB)	(segid 3A4 and resid 382 and name CB)	14.38	0.62	0.63
	assign (segid 3A4 and resid 343 and name CB)	(segid 3A4 and resid 383 and name CA)	17.13	0.48	0.49
	assign (segid 3A4 and resid 343 and name CB)	(segid 3A4 and resid 384 and name CA)	17.31	0.63	0.64
	assign (segid 3A4 and resid 343 and name CB)	(segid 3A4 and resid 384 and name CB)	18.58	0.69	0.69
25	assign (segid 3A4 and resid 343 and name CB)	(segid 3A4 and resid 385 and name CA)	13.94	0.70	0.71
	assign (segid 3A4 and resid 343 and name CB)	(segid 3A4 and resid 386 and name CA)	13.96	0.74	0.73
	assign (segid 3A4 and resid 343 and name CB)	(segid 3A4 and resid 387 and name CA)	14.27	1.16	1.16
	assign (segid 3A4 and resid 343 and name CB)	(segid 3A4 and resid 388 and name CA)	15.73	1.08	1.08
	assign (segid 3A4 and resid 343 and name CB)	(segid 3A4 and resid 388 and name CB)	15.67	1.17	1.16
30	assign (segid 3A4 and resid 343 and name CB)	(segid 3A4 and resid 389 and name CA)	14.61	1.09	1.09
	assign (segid 3A4 and resid 343 and name CB)	(segid 3A4 and resid 389 and name CB)	13.33	1.12	1.13
	assign (segid 3A4 and resid 343 and name CB)	(segid 3A4 and resid 390 and name CA)	16.21	1.09	1.09
	assign (segid 3A4 and resid 343 and name CB)	(segid 3A4 and resid 390 and name CB)	16.98	1.08	1.08
	assign (segid 3A4 and resid 343 and name CB)	(segid 3A4 and resid 391 and name CA)	18.48	0.89	0.90
35	assign (segid 3A4 and resid 343 and name CB)	(segid 3A4 and resid 391 and name CB)	18.85	0.74	0.73
	assign (segid 3A4 and resid 343 and name CB)	(segid 3A4 and resid 431 and name CA)	16.21	1.72	1.71
	assign (segid 3A4 and resid 343 and name CB)	(segid 3A4 and resid 343 and name C)	2.41	0.04	0.04
	assign (segid 3A4 and resid 343 and name N)	(segid 3A4 and resid 343 and name CB)	1.46	0.01	0.01
	assign (segid 3A4 and resid 343 and name N)	(segid 3A4 and resid 343 and name O)	2.48	0.02	0.02
40	assign (segid 3A4 and resid 343 and name N)	(segid 3A4 and resid 344 and name C)	2.79	0.08	0.08
	assign (segid 3A4 and resid 343 and name N)	(segid 3A4 and resid 344 and name CB)	5.73	0.08	0.08
	assign (segid 3A4 and resid 343 and name N)	(segid 3A4 and resid 344 and name N)	4.74	0.05	0.04
	assign (segid 3A4 and resid 343 and name N)	(segid 3A4 and resid 344 and name O)	5.48	0.10	0.11
	assign (segid 3A4 and resid 343 and name N)	(segid 3A4 and resid 344 and name N)	3.49	0.03	0.03
45	assign (segid 3A4 and resid 343 and name N)	(segid 3A4 and resid 344 and name O)	6.14	0.14	0.13
	assign (segid 3A4 and resid 343 and name N)	(segid 3A4 and resid 345 and name CA)	7.65	0.13	0.13
	assign (segid 3A4 and resid 343 and name N)	(segid 3A4 and resid 345 and name N)	6.47	0.11	0.10
	assign (segid 3A4 and resid 343 and name N)	(segid 3A4 and resid 345 and name CB)	3.06	0.05	0.06
	assign (segid 3A4 and resid 343 and name O)	(segid 3A4 and resid 344 and name C)	3.70	0.20	0.20
50	assign (segid 3A4 and resid 343 and name O)	(segid 3A4 and resid 344 and name CB)	2.77	0.02	0.03
	assign (segid 3A4 and resid 343 and name O)	(segid 3A4 and resid 344 and name N)	3.92	0.17	0.17
	assign (segid 3A4 and resid 343 and name O)	(segid 3A4 and resid 344 and name O)	2.25	0.02	0.01
	assign (segid 3A4 and resid 343 and name O)	(segid 3A4 and resid 344 and name O)	4.52	0.26	0.26
	assign (segid 3A4 and resid 343 and name O)	(segid 3A4 and resid 345 and name C)	6.48	0.26	0.26
55	assign (segid 3A4 and resid 343 and name O)	(segid 3A4 and resid 345 and name CA)	5.38	0.30	0.29
	assign (segid 3A4 and resid 343 and name O)	(segid 3A4 and resid 345 and name CB)	5.65	0.44	0.44
	assign (segid 3A4 and resid 343 and name O)	(segid 3A4 and resid 345 and name N)	4.10	0.23	0.23
	assign (segid 3A4 and resid 343 and name O)	(segid 3A4 and resid 345 and name O)	6.77	0.22	0.22
	assign (segid 3A4 and resid 343 and name O)	(segid 3A4 and resid 346 and name N)	7.36	0.32	0.32
60	assign (segid 3A4 and resid 344 and name C)	(segid 3A4 and resid 344 and name CB)	2.52	0.03	0.04
	assign (segid 3A4 and resid 344 and name C)	(segid 3A4 and resid 344 and name O)	1.23	0.01	0.01
	assign (segid 3A4 and resid 344 and name C)	(segid 3A4 and resid 345 and name C)	3.30	0.10	0.11
	assign (segid 3A4 and resid 344 and name C)	(segid 3A4 and resid 345 and name CA)	2.44	0.01	0.02
	assign (segid 3A4 and resid 344 and name C)	(segid 3A4 and resid 345 and name CB)	3.59	0.08	0.08
65	assign (segid 3A4 and resid 344 and name C)	(segid 3A4 and resid 345 and name N)	1.32	0.01	0.01
	assign (segid 3A4 and resid 344 and name C)	(segid 3A4 and resid 345 and name O)	4.00	0.17	0.17
	assign (segid 3A4 and resid 344 and name C)	(segid 3A4 and resid 346 and name C)	6.26	0.11	0.11
	assign (segid 3A4 and resid 344 and name C)	(segid 3A4 and resid 346 and name CA)	5.06	0.14	0.14
	assign (segid 3A4 and resid 344 and name C)	(segid 3A4 and resid 346 and name CB)	5.57	0.23	0.22
70	assign (segid 3A4 and resid 344 and name C)	(segid 3A4 and resid 346 and name N)	3.85	0.11	0.11
	assign (segid 3A4 and resid 344 and name C)	(segid 3A4 and resid 346 and name O)	6.98	0.12	0.12
	assign (segid 3A4 and resid 344 and name C)	(segid 3A4 and resid 347 and name N)	6.73	0.15	0.15
	assign (segid 3A4 and resid 344 and name C)	(segid 3A4 and resid 344 and name C)	1.51	0.01	0.02
	assign (segid 3A4 and resid 344 and name CA)	(segid 3A4 and resid 344 and name CB)	1.53	0.03	0.03
75	assign (segid 3A4 and resid 344 and name CA)	(segid 3A4 and resid 344 and name O)	2.38	0.02	0.01
	assign (segid 3A4 and resid 344 and name CA)	(segid 3A4 and resid 345 and name C)	4.58	0.08	0.09
	assign (segid 3A4 and resid 344 and name CA)	(segid 3A4 and resid 345 and name CB)	3.83	0.02	0.03
	assign (segid 3A4 and resid 344 and name CA)	(segid 3A4 and resid 345 and name N)	4.79	0.09	0.10
	assign (segid 3A4 and resid 344 and name CA)	(segid 3A4 and resid 345 and name O)	2.46	0.04	0.03
80	assign (segid 3A4 and resid 344 and name CA)	(segid 3A4 and resid 345 and name O)	5.04	0.18	0.17
	assign (segid 3A4 and resid 344 and name CA)	(segid 3A4 and resid 346 and name C)	7.50	0.15	0.14
	assign (segid 3A4 and resid 344 and name CA)	(segid 3A4 and resid 346 and name CA)	6.22	0.19	0.20

	assign (segid 3A4 and resid 344 and name CA)	(segid 3A4 and resid 346 and name CB)	6.67	0.32	0.31
	assign (segid 3A4 and resid 344 and name CA)	(segid 3A4 and resid 346 and name N)	5.17	0.15	0.15
	assign (segid 3A4 and resid 344 and name CA)	(segid 3A4 and resid 347 and name CA)	9.21	0.15	0.15
	assign (segid 3A4 and resid 344 and name CA)	(segid 3A4 and resid 347 and name CB)	9.63	0.21	0.22
	assign (segid 3A4 and resid 344 and name CA)	(segid 3A4 and resid 348 and name CA)	11.44	0.27	0.27
5	assign (segid 3A4 and resid 344 and name CA)	(segid 3A4 and resid 349 and name CA)	11.28	0.25	0.25
	assign (segid 3A4 and resid 344 and name CA)	(segid 3A4 and resid 349 and name CB)	10.32	0.28	0.28
	assign (segid 3A4 and resid 344 and name CA)	(segid 3A4 and resid 350 and name CA)	12.11	0.44	0.43
	assign (segid 3A4 and resid 344 and name CA)	(segid 3A4 and resid 350 and name CB)	11.56	0.61	0.62
	assign (segid 3A4 and resid 344 and name CA)	(segid 3A4 and resid 351 and name CA)	14.95	0.32	0.32
10	assign (segid 3A4 and resid 344 and name CA)	(segid 3A4 and resid 352 and name CA)	16.23	0.21	0.21
	assign (segid 3A4 and resid 344 and name CA)	(segid 3A4 and resid 352 and name CB)	15.93	0.32	0.31
	assign (segid 3A4 and resid 344 and name CA)	(segid 3A4 and resid 353 and name CA)	16.32	0.38	0.39
	assign (segid 3A4 and resid 344 and name CA)	(segid 3A4 and resid 353 and name CB)	15.68	0.53	0.53
	assign (segid 3A4 and resid 344 and name CA)	(segid 3A4 and resid 381 and name CA)	16.82	0.56	0.56
15	assign (segid 3A4 and resid 344 and name CA)	(segid 3A4 and resid 382 and name CA)	13.79	0.37	0.37
	assign (segid 3A4 and resid 344 and name CA)	(segid 3A4 and resid 382 and name CB)	12.59	0.43	0.43
	assign (segid 3A4 and resid 344 and name CA)	(segid 3A4 and resid 383 and name CA)	14.38	0.30	0.30
	assign (segid 3A4 and resid 344 and name CA)	(segid 3A4 and resid 384 and name CA)	15.10	0.14	0.14
	assign (segid 3A4 and resid 344 and name CA)	(segid 3A4 and resid 384 and name CB)	16.53	0.47	0.46
20	assign (segid 3A4 and resid 344 and name CA)	(segid 3A4 and resid 385 and name CA)	12.30	0.56	0.57
	assign (segid 3A4 and resid 344 and name CA)	(segid 3A4 and resid 386 and name CA)	13.51	0.55	0.56
	assign (segid 3A4 and resid 344 and name CA)	(segid 3A4 and resid 387 and name CA)	14.83	0.97	0.97
	assign (segid 3A4 and resid 344 and name CA)	(segid 3A4 and resid 388 and name CA)	16.47	0.73	0.72
	assign (segid 3A4 and resid 344 and name CA)	(segid 3A4 and resid 388 and name CB)	16.75	0.79	0.80
25	assign (segid 3A4 and resid 344 and name CA)	(segid 3A4 and resid 389 and name CA)	14.49	0.72	0.71
	assign (segid 3A4 and resid 344 and name CA)	(segid 3A4 and resid 389 and name CB)	13.22	0.72	0.72
	assign (segid 3A4 and resid 344 and name CA)	(segid 3A4 and resid 390 and name CA)	15.40	0.83	0.82
	assign (segid 3A4 and resid 344 and name CA)	(segid 3A4 and resid 390 and name CB)	16.32	0.85	0.85
	assign (segid 3A4 and resid 344 and name CA)	(segid 3A4 and resid 391 and name CA)	16.90	0.62	0.62
30	assign (segid 3A4 and resid 344 and name CA)	(segid 3A4 and resid 391 and name CB)	16.95	0.49	0.48
	assign (segid 3A4 and resid 344 and name CA)	(segid 3A4 and resid 429 and name CA)	15.66	1.56	1.57
	assign (segid 3A4 and resid 344 and name CA)	(segid 3A4 and resid 430 and name CA)	13.04	2.18	2.17
	assign (segid 3A4 and resid 344 and name CA)	(segid 3A4 and resid 431 and name CA)	11.98	1.69	1.69
	assign (segid 3A4 and resid 344 and name CA)	(segid 3A4 and resid 433 and name CA)	15.99	0.78	0.79
35	assign (segid 3A4 and resid 344 and name CA)	(segid 3A4 and resid 345 and name C)	5.15	0.11	0.12
	assign (segid 3A4 and resid 344 and name CB)	(segid 3A4 and resid 345 and name CA)	4.77	0.03	0.04
	assign (segid 3A4 and resid 344 and name CB)	(segid 3A4 and resid 345 and name CB)	5.95	0.05	0.05
	assign (segid 3A4 and resid 344 and name CB)	(segid 3A4 and resid 345 and name N)	3.53	0.03	0.03
	assign (segid 3A4 and resid 344 and name CB)	(segid 3A4 and resid 345 and name O)	5.55	0.25	0.26
40	assign (segid 3A4 and resid 344 and name CB)	(segid 3A4 and resid 346 and name CA)	6.29	0.22	0.23
	assign (segid 3A4 and resid 344 and name CB)	(segid 3A4 and resid 346 and name CB)	6.48	0.40	0.40
	assign (segid 3A4 and resid 344 and name CB)	(segid 3A4 and resid 346 and name N)	5.49	0.17	0.18
	assign (segid 3A4 and resid 344 and name CB)	(segid 3A4 and resid 347 and name CA)	9.55	0.11	0.11
	assign (segid 3A4 and resid 344 and name CB)	(segid 3A4 and resid 347 and name CB)	10.02	0.19	0.19
45	assign (segid 3A4 and resid 344 and name CB)	(segid 3A4 and resid 348 and name CA)	11.32	0.31	0.31
	assign (segid 3A4 and resid 344 and name CB)	(segid 3A4 and resid 349 and name CA)	11.19	0.37	0.37
	assign (segid 3A4 and resid 344 and name CB)	(segid 3A4 and resid 349 and name CB)	10.19	0.43	0.43
	assign (segid 3A4 and resid 344 and name CB)	(segid 3A4 and resid 350 and name CA)	12.47	0.48	0.48
	assign (segid 3A4 and resid 344 and name CB)	(segid 3A4 and resid 350 and name CB)	12.08	0.63	0.63
50	assign (segid 3A4 and resid 344 and name CB)	(segid 3A4 and resid 351 and name CA)	15.19	0.28	0.29
	assign (segid 3A4 and resid 344 and name CB)	(segid 3A4 and resid 352 and name CA)	16.21	0.30	0.30
	assign (segid 3A4 and resid 344 and name CB)	(segid 3A4 and resid 352 and name CB)	15.77	0.40	0.41
	assign (segid 3A4 and resid 344 and name CB)	(segid 3A4 and resid 353 and name CA)	16.50	0.49	0.50
	assign (segid 3A4 and resid 344 and name CB)	(segid 3A4 and resid 353 and name CB)	15.98	0.64	0.64
55	assign (segid 3A4 and resid 344 and name CB)	(segid 3A4 and resid 381 and name CA)	17.44	0.51	0.51
	assign (segid 3A4 and resid 344 and name CB)	(segid 3A4 and resid 382 and name CA)	14.51	0.31	0.32
	assign (segid 3A4 and resid 344 and name CB)	(segid 3A4 and resid 382 and name CB)	13.37	0.38	0.38
	assign (segid 3A4 and resid 344 and name CB)	(segid 3A4 and resid 383 and name CA)	14.83	0.23	0.24
	assign (segid 3A4 and resid 344 and name CB)	(segid 3A4 and resid 384 and name CA)	15.76	0.43	0.43
60	assign (segid 3A4 and resid 344 and name CB)	(segid 3A4 and resid 384 and name CB)	17.22	0.45	0.45
	assign (segid 3A4 and resid 344 and name CB)	(segid 3A4 and resid 385 and name CA)	13.21	0.56	0.56
	assign (segid 3A4 and resid 344 and name CB)	(segid 3A4 and resid 386 and name CA)	14.69	0.54	0.53
	assign (segid 3A4 and resid 344 and name CB)	(segid 3A4 and resid 387 and name CA)	16.16	0.95	0.96
	assign (segid 3A4 and resid 344 and name CB)	(segid 3A4 and resid 388 and name CA)	17.78	0.71	0.71
65	assign (segid 3A4 and resid 344 and name CB)	(segid 3A4 and resid 388 and name CB)	18.09	0.75	0.76
	assign (segid 3A4 and resid 344 and name CB)	(segid 3A4 and resid 389 and name CA)	15.63	0.75	0.75
	assign (segid 3A4 and resid 344 and name CB)	(segid 3A4 and resid 389 and name CB)	14.35	0.75	0.76
	assign (segid 3A4 and resid 344 and name CB)	(segid 3A4 and resid 390 and name CA)	16.44	0.86	0.85
	assign (segid 3A4 and resid 344 and name CB)	(segid 3A4 and resid 390 and name CB)	17.40	0.86	0.86
70	assign (segid 3A4 and resid 344 and name CB)	(segid 3A4 and resid 391 and name CA)	17.70	0.66	0.66
	assign (segid 3A4 and resid 344 and name CB)	(segid 3A4 and resid 391 and name CB)	17.66	0.53	0.52
	assign (segid 3A4 and resid 344 and name CB)	(segid 3A4 and resid 428 and name CA)	17.03	1.44	1.43
	assign (segid 3A4 and resid 344 and name CB)	(segid 3A4 and resid 429 and name CA)	14.60	1.52	1.52
	assign (segid 3A4 and resid 344 and name CB)	(segid 3A4 and resid 430 and name CA)	11.99	2.12	2.13
75	assign (segid 3A4 and resid 344 and name CB)	(segid 3A4 and resid 431 and name CA)	11.27	1.53	1.54
	assign (segid 3A4 and resid 344 and name CB)	(segid 3A4 and resid 433 and name CA)	15.32	0.80	0.80
	assign (segid 3A4 and resid 344 and name CB)	(segid 3A4 and resid 344 and name C)	2.40	0.03	0.02
	assign (segid 3A4 and resid 344 and name N)	(segid 3A4 and resid 344 and name CA)	1.46	0.02	0.01
	assign (segid 3A4 and resid 344 and name N)	(segid 3A4 and resid 344 and name CB)	2.42	0.06	0.06
80	assign (segid 3A4 and resid 344 and name N)	(segid 3A4 and resid 344 and name O)	2.83	0.06	0.06
	assign (segid 3A4 and resid 344 and name N)	(segid 3A4 and resid 345 and name C)	5.67	0.10	0.10
	assign (segid 3A4 and resid 344 and name N)	(segid 3A4 and resid 345 and name CA)	4.67	0.07	0.06

	assign (segid 3A4 and resid 344 and name N) (segid 3A4 and resid 345 and name CB)	5.47	0.14	0.14
	assign (segid 3A4 and resid 344 and name N) (segid 3A4 and resid 345 and name N)	3.42	0.07	0.08
	assign (segid 3A4 and resid 344 and name N) (segid 3A4 and resid 345 and name O)	6.26	0.18	0.17
	assign (segid 3A4 and resid 344 and name N) (segid 3A4 and resid 346 and name CA)	7.38	0.14	0.14
	assign (segid 3A4 and resid 344 and name N) (segid 3A4 and resid 346 and name N)	6.21	0.10	0.10
5	assign (segid 3A4 and resid 344 and name N) (segid 3A4 and resid 346 and name CB)	3.01	0.09	0.08
	assign (segid 3A4 and resid 344 and name O) (segid 3A4 and resid 345 and name C)	3.55	0.19	0.18
	assign (segid 3A4 and resid 344 and name O) (segid 3A4 and resid 345 and name CA)	2.74	0.05	0.05
	assign (segid 3A4 and resid 344 and name O) (segid 3A4 and resid 345 and name CB)	4.01	0.12	0.12
	assign (segid 3A4 and resid 344 and name O) (segid 3A4 and resid 345 and name N)	2.21	0.04	0.04
10	assign (segid 3A4 and resid 344 and name O) (segid 3A4 and resid 345 and name O)	4.48	0.21	0.22
	assign (segid 3A4 and resid 344 and name O) (segid 3A4 and resid 346 and name C)	6.17	0.23	0.23
	assign (segid 3A4 and resid 344 and name O) (segid 3A4 and resid 346 and name CA)	4.95	0.25	0.26
	assign (segid 3A4 and resid 344 and name O) (segid 3A4 and resid 346 and name CB)	5.19	0.31	0.31
	assign (segid 3A4 and resid 344 and name O) (segid 3A4 and resid 346 and name N)	3.72	0.20	0.20
15	assign (segid 3A4 and resid 344 and name O) (segid 3A4 and resid 346 and name O)	6.72	0.19	0.19
	assign (segid 3A4 and resid 344 and name O) (segid 3A4 and resid 347 and name N)	6.86	0.26	0.27
	assign (segid 3A4 and resid 344 and name O) (segid 3A4 and resid 347 and name CB)	2.50	0.05	0.04
	assign (segid 3A4 and resid 345 and name C) (segid 3A4 and resid 345 and name O)	1.23	0.02	0.01
	assign (segid 3A4 and resid 345 and name C) (segid 3A4 and resid 346 and name C)	3.19	0.04	0.05
20	assign (segid 3A4 and resid 345 and name C) (segid 3A4 and resid 346 and name CA)	2.43	0.01	0.01
	assign (segid 3A4 and resid 345 and name C) (segid 3A4 and resid 346 and name CB)	3.62	0.04	0.05
	assign (segid 3A4 and resid 345 and name C) (segid 3A4 and resid 346 and name N)	1.33	0.01	0.00
	assign (segid 3A4 and resid 345 and name C) (segid 3A4 and resid 346 and name O)	4.05	0.14	0.14
	assign (segid 3A4 and resid 345 and name C) (segid 3A4 and resid 347 and name C)	5.88	0.08	0.09
25	assign (segid 3A4 and resid 345 and name C) (segid 3A4 and resid 347 and name CA)	4.75	0.11	0.11
	assign (segid 3A4 and resid 345 and name C) (segid 3A4 and resid 347 and name CB)	5.39	0.15	0.15
	assign (segid 3A4 and resid 345 and name C) (segid 3A4 and resid 347 and name N)	3.51	0.11	0.10
	assign (segid 3A4 and resid 345 and name C) (segid 3A4 and resid 347 and name O)	6.78	0.12	0.13
	assign (segid 3A4 and resid 345 and name C) (segid 3A4 and resid 348 and name C)	7.71	0.14	0.13
30	assign (segid 3A4 and resid 345 and name C) (segid 3A4 and resid 348 and name CA)	7.41	0.14	0.14
	assign (segid 3A4 and resid 345 and name C) (segid 3A4 and resid 348 and name N)	6.13	0.15	0.15
	assign (segid 3A4 and resid 345 and name C) (segid 3A4 and resid 348 and name O)	7.87	0.05	0.06
	assign (segid 3A4 and resid 345 and name C) (segid 3A4 and resid 349 and name CA)	7.51	0.14	0.13
	assign (segid 3A4 and resid 345 and name C) (segid 3A4 and resid 349 and name CB)	6.91	0.17	0.17
35	assign (segid 3A4 and resid 345 and name C) (segid 3A4 and resid 349 and name N)	6.89	0.15	0.15
	assign (segid 3A4 and resid 345 and name C) (segid 3A4 and resid 349 and name O)	7.19	0.18	0.18
	assign (segid 3A4 and resid 345 and name C) (segid 3A4 and resid 350 and name N)	1.52	0.01	0.02
	assign (segid 3A4 and resid 345 and name CA) (segid 3A4 and resid 345 and name CB)	1.53	0.02	0.02
	assign (segid 3A4 and resid 345 and name CA) (segid 3A4 and resid 345 and name O)	2.40	0.02	0.01
40	assign (segid 3A4 and resid 345 and name CA) (segid 3A4 and resid 346 and name C)	4.54	0.05	0.04
	assign (segid 3A4 and resid 345 and name CA) (segid 3A4 and resid 346 and name CA)	3.80	0.03	0.02
	assign (segid 3A4 and resid 345 and name CA) (segid 3A4 and resid 346 and name CB)	4.76	0.07	0.07
	assign (segid 3A4 and resid 345 and name CA) (segid 3A4 and resid 346 and name N)	2.42	0.03	0.03
	assign (segid 3A4 and resid 345 and name CA) (segid 3A4 and resid 346 and name O)	5.20	0.11	0.12
45	assign (segid 3A4 and resid 345 and name CA) (segid 3A4 and resid 347 and name C)	7.20	0.13	0.13
	assign (segid 3A4 and resid 345 and name CA) (segid 3A4 and resid 347 and name CA)	5.99	0.17	0.18
	assign (segid 3A4 and resid 345 and name CA) (segid 3A4 and resid 347 and name CB)	6.58	0.23	0.24
	assign (segid 3A4 and resid 345 and name CA) (segid 3A4 and resid 347 and name N)	4.88	0.15	0.15
	assign (segid 3A4 and resid 345 and name CA) (segid 3A4 and resid 348 and name CA)	8.83	0.11	0.11
50	assign (segid 3A4 and resid 345 and name CA) (segid 3A4 and resid 348 and name N)	7.56	0.13	0.13
	assign (segid 3A4 and resid 345 and name CA) (segid 3A4 and resid 348 and name O)	8.62	0.14	0.14
	assign (segid 3A4 and resid 345 and name CA) (segid 3A4 and resid 349 and name CB)	7.90	0.18	0.17
	assign (segid 3A4 and resid 345 and name CA) (segid 3A4 and resid 350 and name CA)	8.68	0.41	0.41
	assign (segid 3A4 and resid 345 and name CA) (segid 3A4 and resid 350 and name CB)	7.95	0.61	0.62
55	assign (segid 3A4 and resid 345 and name CA) (segid 3A4 and resid 351 and name CA)	11.58	0.42	0.43
	assign (segid 3A4 and resid 345 and name CA) (segid 3A4 and resid 352 and name CA)	13.26	0.18	0.18
	assign (segid 3A4 and resid 345 and name CA) (segid 3A4 and resid 352 and name CB)	13.20	0.23	0.23
	assign (segid 3A4 and resid 345 and name CA) (segid 3A4 and resid 353 and name CA)	13.26	0.25	0.26
	assign (segid 3A4 and resid 345 and name CA) (segid 3A4 and resid 353 and name CB)	12.49	0.38	0.39
60	assign (segid 3A4 and resid 345 and name CA) (segid 3A4 and resid 354 and name CA)	16.99	0.24	0.23
	assign (segid 3A4 and resid 345 and name CA) (segid 3A4 and resid 354 and name CB)	17.73	0.18	0.18
	assign (segid 3A4 and resid 345 and name CA) (segid 3A4 and resid 355 and name CA)	17.31	0.64	0.64
	assign (segid 3A4 and resid 345 and name CA) (segid 3A4 and resid 355 and name CB)	16.72	0.83	0.82
	assign (segid 3A4 and resid 345 and name CA) (segid 3A4 and resid 356 and name CA)	16.50	0.54	0.54
65	assign (segid 3A4 and resid 345 and name CA) (segid 3A4 and resid 356 and name CB)	15.12	0.53	0.54
	assign (segid 3A4 and resid 345 and name CA) (segid 3A4 and resid 357 and name CA)	17.95	0.40	0.40
	assign (segid 3A4 and resid 345 and name CA) (segid 3A4 and resid 357 and name CB)	17.19	0.41	0.42
	assign (segid 3A4 and resid 345 and name CA) (segid 3A4 and resid 360 and name CA)	18.17	0.09	0.10
	assign (segid 3A4 and resid 345 and name CA) (segid 3A4 and resid 360 and name CB)	17.00	0.14	0.14
70	assign (segid 3A4 and resid 345 and name CA) (segid 3A4 and resid 361 and name CA)	19.36	0.14	0.14
	assign (segid 3A4 and resid 345 and name CA) (segid 3A4 and resid 361 and name CB)	19.68	0.14	0.15
	assign (segid 3A4 and resid 345 and name CA) (segid 3A4 and resid 381 and name CA)	13.20	0.61	0.61
	assign (segid 3A4 and resid 345 and name CA) (segid 3A4 and resid 382 and name CA)	10.30	0.40	0.40
	assign (segid 3A4 and resid 345 and name CA) (segid 3A4 and resid 382 and name CB)	9.02	0.43	0.42
75	assign (segid 3A4 and resid 345 and name CA) (segid 3A4 and resid 383 and name CA)	11.37	0.35	0.36
	assign (segid 3A4 and resid 345 and name CA) (segid 3A4 and resid 384 and name CA)	12.39	0.34	0.34
	assign (segid 3A4 and resid 345 and name CA) (segid 3A4 and resid 384 and name CB)	13.79	0.35	0.35
	assign (segid 3A4 and resid 345 and name CA) (segid 3A4 and resid 385 and name CA)	9.53	0.39	0.38
	assign (segid 3A4 and resid 345 and name CA) (segid 3A4 and resid 386 and name CA)	10.65	0.24	0.24
80	assign (segid 3A4 and resid 345 and name CA) (segid 3A4 and resid 387 and name CA)	12.48	0.82	0.83
	assign (segid 3A4 and resid 345 and name CA) (segid 3A4 and resid 388 and name CA)	14.76	0.68	0.67
	assign (segid 3A4 and resid 345 and name CA) (segid 3A4 and resid 388 and name CB)	15.29	0.84	0.84

	assign (segid 3A4 and resid 345 and name CA)	(segid 3A4 and resid 389 and name CA)	13.06	0.44	0.44
	assign (segid 3A4 and resid 345 and name CA)	(segid 3A4 and resid 389 and name CB)	12.05	0.46	0.46
	assign (segid 3A4 and resid 345 and name CA)	(segid 3A4 and resid 390 and name CA)	13.20	0.49	0.49
	assign (segid 3A4 and resid 345 and name CA)	(segid 3A4 and resid 390 and name CB)	13.89	0.55	0.55
	assign (segid 3A4 and resid 345 and name CA)	(segid 3A4 and resid 391 and name CA)	14.92	0.39	0.38
5	assign (segid 3A4 and resid 345 and name CA)	(segid 3A4 and resid 391 and name CB)	14.85	0.33	0.32
	assign (segid 3A4 and resid 345 and name CA)	(segid 3A4 and resid 392 and name CA)	18.47	0.41	0.41
	assign (segid 3A4 and resid 345 and name CA)	(segid 3A4 and resid 392 and name CB)	19.03	0.45	0.45
	assign (segid 3A4 and resid 345 and name CA)	(segid 3A4 and resid 394 and name CA)	18.75	0.43	0.42
	assign (segid 3A4 and resid 345 and name CA)	(segid 3A4 and resid 394 and name CB)	18.02	0.48	0.49
10	assign (segid 3A4 and resid 345 and name CA)	(segid 3A4 and resid 429 and name CA)	16.22	1.37	1.38
	assign (segid 3A4 and resid 345 and name CA)	(segid 3A4 and resid 430 and name CA)	13.92	2.09	2.09
	assign (segid 3A4 and resid 345 and name CA)	(segid 3A4 and resid 431 and name CA)	12.52	1.68	1.68
	assign (segid 3A4 and resid 345 and name CA)	(segid 3A4 and resid 433 and name CA)	15.35	0.54	0.55
	assign (segid 3A4 and resid 345 and name CA)	(segid 3A4 and resid 434 and name CA)	18.62	0.82	0.83
15	assign (segid 3A4 and resid 345 and name CB)	(segid 3A4 and resid 346 and name C)	5.12	0.17	0.17
	assign (segid 3A4 and resid 345 and name CB)	(segid 3A4 and resid 346 and name CA)	4.77	0.11	0.12
	assign (segid 3A4 and resid 345 and name CB)	(segid 3A4 and resid 346 and name CB)	5.92	0.10	0.10
	assign (segid 3A4 and resid 345 and name CB)	(segid 3A4 and resid 346 and name N)	3.53	0.10	0.11
	assign (segid 3A4 and resid 345 and name CB)	(segid 3A4 and resid 346 and name O)	5.73	0.16	0.16
20	assign (segid 3A4 and resid 345 and name CB)	(segid 3A4 and resid 347 and name C)	7.40	0.28	0.27
	assign (segid 3A4 and resid 345 and name CB)	(segid 3A4 and resid 347 and name CA)	6.03	0.32	0.32
	assign (segid 3A4 and resid 345 and name CB)	(segid 3A4 and resid 347 and name CB)	6.42	0.40	0.40
	assign (segid 3A4 and resid 345 and name CB)	(segid 3A4 and resid 347 and name N)	5.20	0.28	0.28
	assign (segid 3A4 and resid 345 and name CB)	(segid 3A4 and resid 348 and name CA)	9.32	0.19	0.19
25	assign (segid 3A4 and resid 345 and name CB)	(segid 3A4 and resid 349 and name CA)	9.30	0.18	0.19
	assign (segid 3A4 and resid 345 and name CB)	(segid 3A4 and resid 349 and name CB)	8.73	0.23	0.23
	assign (segid 3A4 and resid 345 and name CB)	(segid 3A4 and resid 350 and name CA)	8.79	0.49	0.49
	assign (segid 3A4 and resid 345 and name CB)	(segid 3A4 and resid 350 and name CB)	7.85	0.72	0.71
	assign (segid 3A4 and resid 345 and name CB)	(segid 3A4 and resid 351 and name CA)	11.61	0.66	0.65
30	assign (segid 3A4 and resid 345 and name CB)	(segid 3A4 and resid 352 and name CA)	13.64	0.34	0.33
	assign (segid 3A4 and resid 345 and name CB)	(segid 3A4 and resid 352 and name CB)	13.72	0.28	0.28
	assign (segid 3A4 and resid 345 and name CB)	(segid 3A4 and resid 353 and name CA)	13.55	0.30	0.30
	assign (segid 3A4 and resid 345 and name CB)	(segid 3A4 and resid 353 and name CB)	12.67	0.35	0.35
	assign (segid 3A4 and resid 345 and name CB)	(segid 3A4 and resid 354 and name CA)	17.28	0.28	0.28
35	assign (segid 3A4 and resid 345 and name CB)	(segid 3A4 and resid 354 and name CB)	18.12	0.28	0.28
	assign (segid 3A4 and resid 345 and name CB)	(segid 3A4 and resid 355 and name CA)	17.37	0.57	0.56
	assign (segid 3A4 and resid 345 and name CB)	(segid 3A4 and resid 355 and name CB)	16.77	0.75	0.74
	assign (segid 3A4 and resid 345 and name CB)	(segid 3A4 and resid 356 and name CA)	16.32	0.47	0.48
	assign (segid 3A4 and resid 345 and name CB)	(segid 3A4 and resid 356 and name CB)	14.91	0.47	0.46
40	assign (segid 3A4 and resid 345 and name CB)	(segid 3A4 and resid 357 and name CA)	17.91	0.51	0.50
	assign (segid 3A4 and resid 345 and name CB)	(segid 3A4 and resid 357 and name CB)	17.18	0.56	0.56
	assign (segid 3A4 and resid 345 and name CB)	(segid 3A4 and resid 360 and name CA)	18.49	0.32	0.32
	assign (segid 3A4 and resid 345 and name CB)	(segid 3A4 and resid 360 and name CB)	17.35	0.26	0.26
	assign (segid 3A4 and resid 345 and name CB)	(segid 3A4 and resid 381 and name CA)	12.60	0.74	0.75
45	assign (segid 3A4 and resid 345 and name CB)	(segid 3A4 and resid 382 and name CA)	9.54	0.60	0.60
	assign (segid 3A4 and resid 345 and name CB)	(segid 3A4 and resid 382 and name CB)	8.23	0.61	0.62
	assign (segid 3A4 and resid 345 and name CB)	(segid 3A4 and resid 383 and name CA)	10.85	0.61	0.60
	assign (segid 3A4 and resid 345 and name CB)	(segid 3A4 and resid 384 and name CA)	11.55	0.55	0.54
50	assign (segid 3A4 and resid 345 and name CB)	(segid 3A4 and resid 384 and name CB)	12.89	0.56	0.55
	assign (segid 3A4 and resid 345 and name CB)	(segid 3A4 and resid 385 and name CA)	8.45	0.51	0.52
	assign (segid 3A4 and resid 345 and name CB)	(segid 3A4 and resid 386 and name CA)	9.32	0.25	0.25
	assign (segid 3A4 and resid 345 and name CB)	(segid 3A4 and resid 387 and name CA)	11.05	0.83	0.82
	assign (segid 3A4 and resid 345 and name CB)	(segid 3A4 and resid 388 and name CA)	13.35	0.69	0.69
	assign (segid 3A4 and resid 345 and name CB)	(segid 3A4 and resid 388 and name CB)	13.89	0.87	0.88
55	assign (segid 3A4 and resid 345 and name CB)	(segid 3A4 and resid 389 and name CA)	11.80	0.47	0.47
	assign (segid 3A4 and resid 345 and name CB)	(segid 3A4 and resid 389 and name CB)	10.64	0.50	0.50
	assign (segid 3A4 and resid 345 and name CB)	(segid 3A4 and resid 390 and name CA)	11.96	0.55	0.55
	assign (segid 3A4 and resid 345 and name CB)	(segid 3A4 and resid 390 and name CB)	12.60	0.60	0.61
	assign (segid 3A4 and resid 345 and name CB)	(segid 3A4 and resid 391 and name CA)	13.89	0.49	0.49
60	assign (segid 3A4 and resid 345 and name CB)	(segid 3A4 and resid 391 and name CB)	13.91	0.46	0.45
	assign (segid 3A4 and resid 345 and name CB)	(segid 3A4 and resid 392 and name CA)	17.40	0.52	0.52
	assign (segid 3A4 and resid 345 and name CB)	(segid 3A4 and resid 392 and name CB)	17.97	0.56	0.55
	assign (segid 3A4 and resid 345 and name CB)	(segid 3A4 and resid 393 and name CA)	18.92	0.46	0.45
	assign (segid 3A4 and resid 345 and name CB)	(segid 3A4 and resid 394 and name CA)	17.83	0.58	0.57
65	assign (segid 3A4 and resid 345 and name CB)	(segid 3A4 and resid 394 and name CB)	17.05	0.60	0.59
	assign (segid 3A4 and resid 345 and name CB)	(segid 3A4 and resid 430 and name CA)	14.81	2.11	2.10
	assign (segid 3A4 and resid 345 and name CB)	(segid 3A4 and resid 431 and name CA)	13.10	1.81	1.81
	assign (segid 3A4 and resid 345 and name CB)	(segid 3A4 and resid 433 and name CA)	15.91	0.61	0.62
	assign (segid 3A4 and resid 345 and name CB)	(segid 3A4 and resid 345 and name C)	2.42	0.04	0.04
70	assign (segid 3A4 and resid 345 and name N)	(segid 3A4 and resid 345 and name CA)	1.46	0.01	0.00
	assign (segid 3A4 and resid 345 and name N)	(segid 3A4 and resid 345 and name CB)	2.44	0.04	0.04
	assign (segid 3A4 and resid 345 and name N)	(segid 3A4 and resid 345 and name O)	2.98	0.08	0.07
	assign (segid 3A4 and resid 345 and name N)	(segid 3A4 and resid 346 and name C)	5.57	0.11	0.11
	assign (segid 3A4 and resid 345 and name N)	(segid 3A4 and resid 346 and name CA)	4.57	0.14	0.15
75	assign (segid 3A4 and resid 345 and name N)	(segid 3A4 and resid 346 and name CB)	5.41	0.21	0.21
	assign (segid 3A4 and resid 345 and name N)	(segid 3A4 and resid 346 and name N)	3.33	0.14	0.13
	assign (segid 3A4 and resid 345 and name N)	(segid 3A4 and resid 346 and name O)	6.36	0.18	0.18
	assign (segid 3A4 and resid 345 and name N)	(segid 3A4 and resid 347 and name CA)	7.07	0.15	0.14
	assign (segid 3A4 and resid 345 and name N)	(segid 3A4 and resid 347 and name CB)	7.52	0.20	0.19
80	assign (segid 3A4 and resid 345 and name N)	(segid 3A4 and resid 347 and name N)	5.86	0.11	0.11
	assign (segid 3A4 and resid 345 and name O)	(segid 3A4 and resid 345 and name CB)	2.91	0.03	0.03
	assign (segid 3A4 and resid 345 and name O)	(segid 3A4 and resid 346 and name C)	3.29	0.11	0.12

	assign (segid 3A4 and resid 345 and name O) (segid 3A4 and resid 346 and name CA)	2.76	0.02	0.03
	assign (segid 3A4 and resid 345 and name O) (segid 3A4 and resid 346 and name CB)	4.15	0.06	0.06
	assign (segid 3A4 and resid 345 and name O) (segid 3A4 and resid 346 and name N)	2.25	0.01	0.00
	assign (segid 3A4 and resid 345 and name O) (segid 3A4 and resid 346 and name O)	4.34	0.21	0.20
	assign (segid 3A4 and resid 345 and name O) (segid 3A4 and resid 347 and name C)	5.57	0.15	0.14
5	assign (segid 3A4 and resid 345 and name O) (segid 3A4 and resid 347 and name CA)	4.34	0.16	0.17
	assign (segid 3A4 and resid 345 and name O) (segid 3A4 and resid 347 and name CB)	4.69	0.16	0.15
	assign (segid 3A4 and resid 345 and name O) (segid 3A4 and resid 347 and name N)	3.16	0.13	0.13
	assign (segid 3A4 and resid 345 and name O) (segid 3A4 and resid 347 and name O)	6.56	0.17	0.16
	assign (segid 3A4 and resid 345 and name O) (segid 3A4 and resid 348 and name CA)	7.14	0.20	0.21
10	assign (segid 3A4 and resid 345 and name O) (segid 3A4 and resid 348 and name N)	5.79	0.20	0.20
	assign (segid 3A4 and resid 345 and name O) (segid 3A4 and resid 349 and name CB)	7.43	0.22	0.21
	assign (segid 3A4 and resid 345 and name O) (segid 3A4 and resid 349 and name N)	7.03	0.21	0.20
	assign (segid 3A4 and resid 345 and name O) (segid 3A4 and resid 350 and name N)	7.50	0.05	0.05
	assign (segid 3A4 and resid 345 and name O) (segid 3A4 and resid 346 and name CB)	2.51	0.02	0.02
15	assign (segid 3A4 and resid 346 and name C) (segid 3A4 and resid 346 and name O)	1.23	0.00	0.00
	assign (segid 3A4 and resid 346 and name C) (segid 3A4 and resid 347 and name C)	3.01	0.03	0.04
	assign (segid 3A4 and resid 346 and name C) (segid 3A4 and resid 347 and name CA)	2.45	0.02	0.01
	assign (segid 3A4 and resid 346 and name C) (segid 3A4 and resid 347 and name CB)	3.73	0.02	0.01
	assign (segid 3A4 and resid 346 and name C) (segid 3A4 and resid 347 and name N)	1.33	0.01	0.01
20	assign (segid 3A4 and resid 346 and name C) (segid 3A4 and resid 347 and name O)	3.89	0.09	0.09
	assign (segid 3A4 and resid 346 and name C) (segid 3A4 and resid 348 and name C)	4.56	0.09	0.09
	assign (segid 3A4 and resid 346 and name C) (segid 3A4 and resid 348 and name CA)	4.38	0.12	0.13
	assign (segid 3A4 and resid 346 and name C) (segid 3A4 and resid 348 and name N)	3.21	0.14	0.14
	assign (segid 3A4 and resid 346 and name C) (segid 3A4 and resid 348 and name O)	5.70	0.09	0.09
25	assign (segid 3A4 and resid 346 and name C) (segid 3A4 and resid 349 and name C)	5.05	0.13	0.13
	assign (segid 3A4 and resid 346 and name C) (segid 3A4 and resid 349 and name CA)	4.64	0.13	0.12
	assign (segid 3A4 and resid 346 and name C) (segid 3A4 and resid 349 and name CB)	4.46	0.19	0.19
	assign (segid 3A4 and resid 346 and name C) (segid 3A4 and resid 349 and name N)	3.84	0.12	0.12
	assign (segid 3A4 and resid 346 and name C) (segid 3A4 and resid 349 and name O)	6.26	0.15	0.14
30	assign (segid 3A4 and resid 346 and name C) (segid 3A4 and resid 350 and name C)	6.51	0.41	0.40
	assign (segid 3A4 and resid 346 and name C) (segid 3A4 and resid 350 and name CA)	5.39	0.37	0.37
	assign (segid 3A4 and resid 346 and name C) (segid 3A4 and resid 350 and name CB)	5.07	0.55	0.55
	assign (segid 3A4 and resid 346 and name C) (segid 3A4 and resid 350 and name N)	4.44	0.29	0.29
	assign (segid 3A4 and resid 346 and name C) (segid 3A4 and resid 351 and name N)	6.39	0.44	0.43
35	assign (segid 3A4 and resid 346 and name C) (segid 3A4 and resid 382 and name O)	7.16	0.47	0.46
	assign (segid 3A4 and resid 346 and name CA) (segid 3A4 and resid 346 and name C)	1.53	0.01	0.00
	assign (segid 3A4 and resid 346 and name CA) (segid 3A4 and resid 346 and name CB)	1.52	0.02	0.02
	assign (segid 3A4 and resid 346 and name CA) (segid 3A4 and resid 346 and name O)	2.41	0.02	0.02
	assign (segid 3A4 and resid 346 and name CA) (segid 3A4 and resid 347 and name C)	4.41	0.03	0.02
40	assign (segid 3A4 and resid 346 and name CA) (segid 3A4 and resid 347 and name CA)	3.81	0.02	0.02
	assign (segid 3A4 and resid 346 and name CA) (segid 3A4 and resid 347 and name CB)	4.86	0.04	0.03
	assign (segid 3A4 and resid 346 and name CA) (segid 3A4 and resid 347 and name N)	2.43	0.02	0.02
	assign (segid 3A4 and resid 346 and name CA) (segid 3A4 and resid 347 and name O)	5.36	0.09	0.09
	assign (segid 3A4 and resid 346 and name CA) (segid 3A4 and resid 348 and name C)	5.58	0.13	0.13
45	assign (segid 3A4 and resid 346 and name CA) (segid 3A4 and resid 348 and name CA)	5.39	0.17	0.16
	assign (segid 3A4 and resid 346 and name CA) (segid 3A4 and resid 348 and name N)	4.32	0.16	0.15
	assign (segid 3A4 and resid 346 and name CA) (segid 3A4 and resid 348 and name O)	6.76	0.13	0.13
	assign (segid 3A4 and resid 346 and name CA) (segid 3A4 and resid 349 and name C)	6.05	0.15	0.15
	assign (segid 3A4 and resid 346 and name CA) (segid 3A4 and resid 349 and name CA)	5.41	0.14	0.13
50	assign (segid 3A4 and resid 346 and name CA) (segid 3A4 and resid 349 and name CB)	4.87	0.20	0.19
	assign (segid 3A4 and resid 346 and name CA) (segid 3A4 and resid 349 and name N)	4.71	0.13	0.13
	assign (segid 3A4 and resid 346 and name CA) (segid 3A4 and resid 349 and name O)	7.22	0.13	0.14
	assign (segid 3A4 and resid 346 and name CA) (segid 3A4 and resid 350 and name C)	6.65	0.39	0.38
	assign (segid 3A4 and resid 346 and name CA) (segid 3A4 and resid 350 and name CB)	6.40	0.58	0.58
55	assign (segid 3A4 and resid 346 and name CA) (segid 3A4 and resid 350 and name N)	5.62	0.32	0.32
	assign (segid 3A4 and resid 346 and name CA) (segid 3A4 and resid 351 and name CA)	9.07	0.44	0.45
	assign (segid 3A4 and resid 346 and name CA) (segid 3A4 and resid 352 and name CA)	10.30	0.13	0.13
	assign (segid 3A4 and resid 346 and name CA) (segid 3A4 and resid 352 and name CB)	9.99	0.09	0.08
	assign (segid 3A4 and resid 346 and name CA) (segid 3A4 and resid 353 and name CA)	11.03	0.17	0.17
60	assign (segid 3A4 and resid 346 and name CA) (segid 3A4 and resid 353 and name CB)	10.62	0.21	0.22
	assign (segid 3A4 and resid 346 and name CA) (segid 3A4 and resid 354 and name CA)	14.75	0.21	0.21
	assign (segid 3A4 and resid 346 and name CA) (segid 3A4 and resid 354 and name CB)	15.43	0.31	0.31
	assign (segid 3A4 and resid 346 and name CA) (segid 3A4 and resid 355 and name CA)	15.80	0.34	0.33
	assign (segid 3A4 and resid 346 and name CA) (segid 3A4 and resid 355 and name CB)	15.47	0.51	0.50
65	assign (segid 3A4 and resid 346 and name CA) (segid 3A4 and resid 356 and name CA)	14.99	0.31	0.31
	assign (segid 3A4 and resid 346 and name CA) (segid 3A4 and resid 356 and name CB)	13.70	0.34	0.35
	assign (segid 3A4 and resid 346 and name CA) (segid 3A4 and resid 357 and name CA)	15.78	0.27	0.27
	assign (segid 3A4 and resid 346 and name CA) (segid 3A4 and resid 357 and name CB)	14.85	0.32	0.32
	assign (segid 3A4 and resid 346 and name CA) (segid 3A4 and resid 358 and name CA)	18.63	0.26	0.26
70	assign (segid 3A4 and resid 346 and name CA) (segid 3A4 and resid 359 and name CA)	18.73	0.35	0.35
	assign (segid 3A4 and resid 346 and name CA) (segid 3A4 and resid 360 and name CA)	15.17	0.28	0.28
	assign (segid 3A4 and resid 346 and name CA) (segid 3A4 and resid 360 and name CB)	14.05	0.34	0.34
	assign (segid 3A4 and resid 346 and name CA) (segid 3A4 and resid 361 and name CA)	15.96	0.25	0.26
	assign (segid 3A4 and resid 346 and name CA) (segid 3A4 and resid 361 and name CB)	16.24	0.25	0.25
75	assign (segid 3A4 and resid 346 and name CA) (segid 3A4 and resid 362 and name CA)	19.04	0.25	0.25
	assign (segid 3A4 and resid 346 and name CA) (segid 3A4 and resid 381 and name CA)	11.89	0.43	0.42
	assign (segid 3A4 and resid 346 and name CA) (segid 3A4 and resid 382 and name CA)	9.53	0.41	0.40
	assign (segid 3A4 and resid 346 and name CA) (segid 3A4 and resid 382 and name CB)	8.50	0.43	0.42
	assign (segid 3A4 and resid 346 and name CA) (segid 3A4 and resid 383 and name CA)	9.96	0.36	0.37
80	assign (segid 3A4 and resid 346 and name CA) (segid 3A4 and resid 384 and name CA)	12.00	0.47	0.46
	assign (segid 3A4 and resid 346 and name CA) (segid 3A4 and resid 384 and name CB)	13.44	0.43	0.44
	assign (segid 3A4 and resid 346 and name CA) (segid 3A4 and resid 385 and name CA)	10.04	0.52	0.53

	assign (segid 3A4 and resid 346 and name CA) (segid 3A4 and resid 386 and name CA)	11.97	0.50	0.51
	assign (segid 3A4 and resid 346 and name CA) (segid 3A4 and resid 387 and name CA)	14.59	0.89	0.89
	assign (segid 3A4 and resid 346 and name CA) (segid 3A4 and resid 388 and name CA)	17.06	0.79	0.80
	assign (segid 3A4 and resid 346 and name CA) (segid 3A4 and resid 389 and name CA)	15.08	0.64	0.64
	assign (segid 3A4 and resid 346 and name CA) (segid 3A4 and resid 389 and name CB)	14.23	0.68	0.68
5	assign (segid 3A4 and resid 346 and name CA) (segid 3A4 and resid 390 and name CA)	14.42	0.49	0.49
	assign (segid 3A4 and resid 346 and name CA) (segid 3A4 and resid 390 and name CB)	15.05	0.49	0.50
	assign (segid 3A4 and resid 346 and name CA) (segid 3A4 and resid 391 and name CA)	15.47	0.52	0.52
	assign (segid 3A4 and resid 346 and name CA) (segid 3A4 and resid 391 and name CB)	15.04	0.56	0.55
	assign (segid 3A4 and resid 346 and name CA) (segid 3A4 and resid 394 and name CA)	18.45	0.54	0.53
10	assign (segid 3A4 and resid 346 and name CA) (segid 3A4 and resid 394 and name CB)	17.85	0.64	0.64
	assign (segid 3A4 and resid 346 and name CA) (segid 3A4 and resid 397 and name CA)	18.99	0.57	0.58
	assign (segid 3A4 and resid 346 and name CA) (segid 3A4 and resid 427 and name CA)	16.90	0.67	0.67
	assign (segid 3A4 and resid 346 and name CA) (segid 3A4 and resid 428 and name CA)	15.90	1.13	1.13
	assign (segid 3A4 and resid 346 and name CA) (segid 3A4 and resid 429 and name CA)	13.98	1.37	1.36
15	assign (segid 3A4 and resid 346 and name CA) (segid 3A4 and resid 430 and name CA)	12.11	2.09	2.10
	assign (segid 3A4 and resid 346 and name CA) (segid 3A4 and resid 431 and name CA)	11.19	1.48	1.47
	assign (segid 3A4 and resid 346 and name CA) (segid 3A4 and resid 433 and name CA)	12.72	0.64	0.63
	assign (segid 3A4 and resid 346 and name CA) (segid 3A4 and resid 434 and name CA)	15.88	0.92	0.91
	assign (segid 3A4 and resid 346 and name CA) (segid 3A4 and resid 347 and name C)	5.09	0.10	0.10
20	assign (segid 3A4 and resid 346 and name CB) (segid 3A4 and resid 347 and name CA)	4.88	0.05	0.05
	assign (segid 3A4 and resid 346 and name CB) (segid 3A4 and resid 347 and name CB)	6.07	0.03	0.04
	assign (segid 3A4 and resid 346 and name CB) (segid 3A4 and resid 347 and name N)	3.65	0.04	0.03
	assign (segid 3A4 and resid 346 and name CB) (segid 3A4 and resid 347 and name O)	5.92	0.13	0.14
	assign (segid 3A4 and resid 346 and name CB) (segid 3A4 and resid 348 and name C)	5.42	0.25	0.24
25	assign (segid 3A4 and resid 346 and name CB) (segid 3A4 and resid 348 and name CA)	5.51	0.28	0.27
	assign (segid 3A4 and resid 346 and name CB) (segid 3A4 and resid 348 and name N)	4.78	0.23	0.22
	assign (segid 3A4 and resid 346 and name CB) (segid 3A4 and resid 348 and name O)	6.55	0.24	0.23
	assign (segid 3A4 and resid 346 and name CB) (segid 3A4 and resid 349 and name C)	5.67	0.22	0.23
	assign (segid 3A4 and resid 346 and name CB) (segid 3A4 and resid 349 and name CA)	4.80	0.23	0.23
30	assign (segid 3A4 and resid 346 and name CB) (segid 3A4 and resid 349 and name CB)	3.97	0.26	0.27
	assign (segid 3A4 and resid 346 and name CB) (segid 3A4 and resid 349 and name N)	4.35	0.23	0.23
	assign (segid 3A4 and resid 346 and name CB) (segid 3A4 and resid 349 and name O)	6.76	0.20	0.21
	assign (segid 3A4 and resid 346 and name CB) (segid 3A4 and resid 350 and name CA)	6.74	0.39	0.39
	assign (segid 3A4 and resid 346 and name CB) (segid 3A4 and resid 350 and name CB)	6.81	0.57	0.56
35	assign (segid 3A4 and resid 346 and name CB) (segid 3A4 and resid 350 and name N)	5.56	0.36	0.36
	assign (segid 3A4 and resid 346 and name CB) (segid 3A4 and resid 351 and name CA)	9.25	0.39	0.39
	assign (segid 3A4 and resid 346 and name CB) (segid 3A4 and resid 352 and name CA)	9.91	0.14	0.13
	assign (segid 3A4 and resid 346 and name CB) (segid 3A4 and resid 352 and name CB)	9.46	0.14	0.13
	assign (segid 3A4 and resid 346 and name CB) (segid 3A4 and resid 353 and name CA)	10.58	0.23	0.23
40	assign (segid 3A4 and resid 346 and name CB) (segid 3A4 and resid 353 and name CB)	10.29	0.28	0.29
	assign (segid 3A4 and resid 346 and name CB) (segid 3A4 and resid 354 and name CA)	14.19	0.28	0.28
	assign (segid 3A4 and resid 346 and name CB) (segid 3A4 and resid 354 and name CB)	14.75	0.37	0.37
	assign (segid 3A4 and resid 346 and name CB) (segid 3A4 and resid 355 and name CA)	15.43	0.36	0.35
	assign (segid 3A4 and resid 346 and name CB) (segid 3A4 and resid 355 and name CB)	15.09	0.50	0.49
45	assign (segid 3A4 and resid 346 and name CB) (segid 3A4 and resid 356 and name CA)	14.94	0.35	0.35
	assign (segid 3A4 and resid 346 and name CB) (segid 3A4 and resid 356 and name CB)	13.74	0.39	0.39
	assign (segid 3A4 and resid 346 and name CB) (segid 3A4 and resid 357 and name CA)	15.66	0.29	0.29
	assign (segid 3A4 and resid 346 and name CB) (segid 3A4 and resid 357 and name CB)	14.76	0.30	0.31
50	assign (segid 3A4 and resid 346 and name CB) (segid 3A4 and resid 358 and name CA)	18.24	0.27	0.27
	assign (segid 3A4 and resid 346 and name CB) (segid 3A4 and resid 359 and name CA)	18.23	0.45	0.44
	assign (segid 3A4 and resid 346 and name CB) (segid 3A4 and resid 360 and name CA)	14.75	0.34	0.34
	assign (segid 3A4 and resid 346 and name CB) (segid 3A4 and resid 360 and name CB)	13.58	0.40	0.41
	assign (segid 3A4 and resid 346 and name CB) (segid 3A4 and resid 361 and name CA)	15.42	0.26	0.26
	assign (segid 3A4 and resid 346 and name CB) (segid 3A4 and resid 361 and name CB)	15.57	0.28	0.28
55	assign (segid 3A4 and resid 346 and name CB) (segid 3A4 and resid 362 and name CA)	18.67	0.25	0.25
	assign (segid 3A4 and resid 346 and name CB) (segid 3A4 and resid 363 and name CA)	19.34	0.35	0.34
	assign (segid 3A4 and resid 346 and name CB) (segid 3A4 and resid 381 and name CA)	12.63	0.47	0.47
	assign (segid 3A4 and resid 346 and name CB) (segid 3A4 and resid 382 and name CA)	10.59	0.46	0.47
	assign (segid 3A4 and resid 346 and name CB) (segid 3A4 and resid 382 and name CB)	9.57	0.47	0.48
60	assign (segid 3A4 and resid 346 and name CB) (segid 3A4 and resid 383 and name CA)	11.04	0.49	0.48
	assign (segid 3A4 and resid 346 and name CB) (segid 3A4 and resid 384 and name CA)	13.30	0.53	0.54
	assign (segid 3A4 and resid 346 and name CB) (segid 3A4 and resid 384 and name CB)	14.74	0.50	0.50
	assign (segid 3A4 and resid 346 and name CB) (segid 3A4 and resid 385 and name CA)	11.46	0.55	0.55
	assign (segid 3A4 and resid 346 and name CB) (segid 3A4 and resid 386 and name CA)	13.32	0.50	0.50
65	assign (segid 3A4 and resid 346 and name CB) (segid 3A4 and resid 387 and name CA)	15.95	0.90	0.91
	assign (segid 3A4 and resid 346 and name CB) (segid 3A4 and resid 389 and name CA)	16.55	0.60	0.60
	assign (segid 3A4 and resid 346 and name CB) (segid 3A4 and resid 389 and name CB)	15.69	0.63	0.62
	assign (segid 3A4 and resid 346 and name CB) (segid 3A4 and resid 390 and name CA)	15.89	0.50	0.49
	assign (segid 3A4 and resid 346 and name CB) (segid 3A4 and resid 390 and name CB)	16.50	0.51	0.51
70	assign (segid 3A4 and resid 346 and name CB) (segid 3A4 and resid 391 and name CA)	16.91	0.55	0.54
	assign (segid 3A4 and resid 346 and name CB) (segid 3A4 and resid 391 and name CB)	16.43	0.60	0.60
	assign (segid 3A4 and resid 346 and name CB) (segid 3A4 and resid 426 and name CA)	18.32	1.05	1.05
	assign (segid 3A4 and resid 346 and name CB) (segid 3A4 and resid 427 and name CA)	16.73	0.59	0.60
	assign (segid 3A4 and resid 346 and name CB) (segid 3A4 and resid 428 and name CA)	15.69	1.01	1.00
75	assign (segid 3A4 and resid 346 and name CB) (segid 3A4 and resid 429 and name CA)	13.86	1.47	1.47
	assign (segid 3A4 and resid 346 and name CB) (segid 3A4 and resid 430 and name CA)	12.13	2.13	2.14
	assign (segid 3A4 and resid 346 and name CB) (segid 3A4 and resid 431 and name CA)	11.63	1.37	1.37
	assign (segid 3A4 and resid 346 and name CB) (segid 3A4 and resid 433 and name CA)	12.93	0.82	0.81
	assign (segid 3A4 and resid 346 and name CB) (segid 3A4 and resid 434 and name CA)	16.08	1.00	1.00
80	assign (segid 3A4 and resid 346 and name N) (segid 3A4 and resid 346 and name C)	2.46	0.04	0.03
	assign (segid 3A4 and resid 346 and name N) (segid 3A4 and resid 346 and name CA)	1.46	0.02	0.01
	assign (segid 3A4 and resid 346 and name N) (segid 3A4 and resid 346 and name CB)	2.40	0.03	0.04

	assign (segid 3A4 and resid 346 and name N)	(segid 3A4 and resid 346 and name O)	3.16	0.08	0.07
	assign (segid 3A4 and resid 346 and name N)	(segid 3A4 and resid 347 and name C)	5.42	0.06	0.06
	assign (segid 3A4 and resid 346 and name N)	(segid 3A4 and resid 347 and name CA)	4.55	0.10	0.10
	assign (segid 3A4 and resid 346 and name N)	(segid 3A4 and resid 347 and name CB)	5.50	0.12	0.13
5	assign (segid 3A4 and resid 346 and name N)	(segid 3A4 and resid 347 and name N)	3.24	0.10	0.09
	assign (segid 3A4 and resid 346 and name N)	(segid 3A4 and resid 347 and name O)	6.28	0.13	0.13
	assign (segid 3A4 and resid 346 and name N)	(segid 3A4 and resid 348 and name C)	6.82	0.10	0.10
	assign (segid 3A4 and resid 346 and name N)	(segid 3A4 and resid 348 and name CA)	6.70	0.12	0.13
	assign (segid 3A4 and resid 346 and name N)	(segid 3A4 and resid 348 and name N)	5.57	0.12	0.12
	assign (segid 3A4 and resid 346 and name N)	(segid 3A4 and resid 349 and name C)	6.84	0.09	0.10
10	assign (segid 3A4 and resid 346 and name N)	(segid 3A4 and resid 349 and name CA)	6.39	0.08	0.08
	assign (segid 3A4 and resid 346 and name N)	(segid 3A4 and resid 349 and name CB)	5.68	0.13	0.14
	assign (segid 3A4 and resid 346 and name N)	(segid 3A4 and resid 349 and name N)	5.89	0.11	0.10
	assign (segid 3A4 and resid 346 and name N)	(segid 3A4 and resid 350 and name CA)	7.12	0.40	0.40
	assign (segid 3A4 and resid 346 and name N)	(segid 3A4 and resid 350 and name CB)	6.70	0.63	0.62
15	assign (segid 3A4 and resid 346 and name N)	(segid 3A4 and resid 350 and name N)	6.30	0.30	0.30
	assign (segid 3A4 and resid 346 and name N)	(segid 3A4 and resid 346 and name CB)	2.84	0.06	0.06
	assign (segid 3A4 and resid 346 and name O)	(segid 3A4 and resid 347 and name C)	2.95	0.10	0.10
	assign (segid 3A4 and resid 346 and name O)	(segid 3A4 and resid 347 and name CA)	2.77	0.04	0.05
	assign (segid 3A4 and resid 346 and name O)	(segid 3A4 and resid 347 and name CB)	4.26	0.05	0.05
20	assign (segid 3A4 and resid 346 and name O)	(segid 3A4 and resid 347 and name N)	2.24	0.03	0.02
	assign (segid 3A4 and resid 346 and name O)	(segid 3A4 and resid 347 and name O)	3.50	0.17	0.16
	assign (segid 3A4 and resid 346 and name O)	(segid 3A4 and resid 348 and name C)	4.03	0.14	0.13
	assign (segid 3A4 and resid 346 and name O)	(segid 3A4 and resid 348 and name CA)	4.25	0.17	0.16
	assign (segid 3A4 and resid 346 and name O)	(segid 3A4 and resid 348 and name N)	3.31	0.15	0.15
25	assign (segid 3A4 and resid 346 and name O)	(segid 3A4 and resid 348 and name O)	5.05	0.11	0.10
	assign (segid 3A4 and resid 346 and name O)	(segid 3A4 and resid 349 and name C)	3.94	0.14	0.14
	assign (segid 3A4 and resid 346 and name O)	(segid 3A4 and resid 349 and name CA)	3.70	0.15	0.15
	assign (segid 3A4 and resid 346 and name O)	(segid 3A4 and resid 349 and name CB)	3.55	0.22	0.21
	assign (segid 3A4 and resid 346 and name O)	(segid 3A4 and resid 349 and name N)	3.15	0.16	0.17
30	assign (segid 3A4 and resid 346 and name O)	(segid 3A4 and resid 349 and name O)	5.12	0.15	0.15
	assign (segid 3A4 and resid 346 and name O)	(segid 3A4 and resid 350 and name C)	5.48	0.40	0.39
	assign (segid 3A4 and resid 346 and name O)	(segid 3A4 and resid 350 and name CA)	4.29	0.37	0.36
	assign (segid 3A4 and resid 346 and name O)	(segid 3A4 and resid 350 and name CB)	4.13	0.53	0.54
35	assign (segid 3A4 and resid 346 and name O)	(segid 3A4 and resid 350 and name N)	3.31	0.31	0.30
	assign (segid 3A4 and resid 346 and name O)	(segid 3A4 and resid 350 and name O)	6.59	0.36	0.37
	assign (segid 3A4 and resid 346 and name O)	(segid 3A4 and resid 351 and name CA)	6.84	0.42	0.43
	assign (segid 3A4 and resid 346 and name O)	(segid 3A4 and resid 351 and name N)	5.49	0.41	0.42
	assign (segid 3A4 and resid 346 and name O)	(segid 3A4 and resid 351 and name O)	7.20	0.25	0.25
	assign (segid 3A4 and resid 346 and name O)	(segid 3A4 and resid 352 and name N)	2.51	0.03	0.02
40	assign (segid 3A4 and resid 347 and name C)	(segid 3A4 and resid 347 and name CB)	1.23	0.01	0.01
	assign (segid 3A4 and resid 347 and name C)	(segid 3A4 and resid 347 and name O)	1.23	0.01	0.01
	assign (segid 3A4 and resid 347 and name C)	(segid 3A4 and resid 348 and name C)	3.01	0.10	0.10
	assign (segid 3A4 and resid 347 and name C)	(segid 3A4 and resid 348 and name CA)	2.44	0.03	0.03
	assign (segid 3A4 and resid 347 and name C)	(segid 3A4 and resid 348 and name N)	1.33	0.01	0.01
	assign (segid 3A4 and resid 347 and name C)	(segid 3A4 and resid 348 and name O)	3.90	0.12	0.13
45	assign (segid 3A4 and resid 347 and name C)	(segid 3A4 and resid 349 and name C)	4.54	0.15	0.14
	assign (segid 3A4 and resid 347 and name C)	(segid 3A4 and resid 349 and name CA)	4.43	0.15	0.16
	assign (segid 3A4 and resid 347 and name C)	(segid 3A4 and resid 349 and name CB)	5.20	0.17	0.18
	assign (segid 3A4 and resid 347 and name C)	(segid 3A4 and resid 349 and name N)	3.26	0.15	0.15
	assign (segid 3A4 and resid 347 and name C)	(segid 3A4 and resid 349 and name O)	5.64	0.17	0.16
50	assign (segid 3A4 and resid 347 and name C)	(segid 3A4 and resid 350 and name C)	5.07	0.41	0.41
	assign (segid 3A4 and resid 347 and name C)	(segid 3A4 and resid 350 and name CA)	4.61	0.25	0.25
	assign (segid 3A4 and resid 347 and name C)	(segid 3A4 and resid 350 and name CB)	4.38	0.28	0.28
	assign (segid 3A4 and resid 347 and name C)	(segid 3A4 and resid 350 and name N)	3.85	0.20	0.20
	assign (segid 3A4 and resid 347 and name C)	(segid 3A4 and resid 350 and name O)	6.26	0.40	0.41
55	assign (segid 3A4 and resid 347 and name C)	(segid 3A4 and resid 351 and name C)	6.38	0.50	0.51
	assign (segid 3A4 and resid 347 and name C)	(segid 3A4 and resid 351 and name CA)	5.36	0.58	0.58
	assign (segid 3A4 and resid 347 and name C)	(segid 3A4 and resid 351 and name N)	4.41	0.49	0.48
	assign (segid 3A4 and resid 347 and name C)	(segid 3A4 and resid 352 and name CG)	7.32	0.19	0.18
	assign (segid 3A4 and resid 347 and name C)	(segid 3A4 and resid 352 and name N)	6.34	0.43	0.43
60	assign (segid 3A4 and resid 347 and name C)	(segid 3A4 and resid 382 and name C)	5.82	0.67	0.67
	assign (segid 3A4 and resid 347 and name C)	(segid 3A4 and resid 382 and name CA)	6.30	0.65	0.64
	assign (segid 3A4 and resid 347 and name C)	(segid 3A4 and resid 382 and name CB)	5.75	0.69	0.70
	assign (segid 3A4 and resid 347 and name C)	(segid 3A4 and resid 382 and name N)	6.44	0.55	0.56
	assign (segid 3A4 and resid 347 and name C)	(segid 3A4 and resid 382 and name O)	5.41	0.68	0.67
65	assign (segid 3A4 and resid 347 and name C)	(segid 3A4 and resid 383 and name CA)	6.36	0.60	0.60
	assign (segid 3A4 and resid 347 and name C)	(segid 3A4 and resid 383 and name N)	6.31	0.63	0.63
	assign (segid 3A4 and resid 347 and name CA)	(segid 3A4 and resid 347 and name C)	1.53	0.01	0.00
	assign (segid 3A4 and resid 347 and name CA)	(segid 3A4 and resid 347 and name CB)	1.54	0.02	0.01
	assign (segid 3A4 and resid 347 and name CA)	(segid 3A4 and resid 347 and name O)	2.38	0.03	0.03
70	assign (segid 3A4 and resid 347 and name CA)	(segid 3A4 and resid 348 and name C)	4.42	0.10	0.10
	assign (segid 3A4 and resid 347 and name CA)	(segid 3A4 and resid 348 and name CA)	3.83	0.05	0.06
	assign (segid 3A4 and resid 347 and name CA)	(segid 3A4 and resid 348 and name N)	2.46	0.07	0.07
	assign (segid 3A4 and resid 347 and name CA)	(segid 3A4 and resid 348 and name O)	5.37	0.13	0.13
	assign (segid 3A4 and resid 347 and name CA)	(segid 3A4 and resid 349 and name C)	5.46	0.18	0.19
75	assign (segid 3A4 and resid 347 and name CA)	(segid 3A4 and resid 349 and name CA)	5.43	0.18	0.17
	assign (segid 3A4 and resid 347 and name CA)	(segid 3A4 and resid 349 and name CB)	5.88	0.23	0.22
	assign (segid 3A4 and resid 347 and name CA)	(segid 3A4 and resid 349 and name N)	4.37	0.16	0.15
	assign (segid 3A4 and resid 347 and name CA)	(segid 3A4 and resid 349 and name O)	6.61	0.22	0.21
80	assign (segid 3A4 and resid 347 and name CA)	(segid 3A4 and resid 350 and name C)	5.86	0.49	0.50
	assign (segid 3A4 and resid 347 and name CA)	(segid 3A4 and resid 350 and name CA)	5.16	0.34	0.35
	assign (segid 3A4 and resid 347 and name CA)	(segid 3A4 and resid 350 and name CB)	4.53	0.44	0.44
	assign (segid 3A4 and resid 347 and name CA)	(segid 3A4 and resid 350 and name N)	4.57	0.26	0.27

	assign (segid 3A4 and resid 347 and name CA)	(segid 3A4 and resid 351 and name CA)	6.47	0.63	0.64
	assign (segid 3A4 and resid 347 and name CA)	(segid 3A4 and resid 351 and name N)	5.42	0.55	0.55
	assign (segid 3A4 and resid 347 and name CA)	(segid 3A4 and resid 352 and name CA)	8.88	0.38	0.37
	assign (segid 3A4 and resid 347 and name CA)	(segid 3A4 and resid 352 and name CB)	8.91	0.29	0.30
5	assign (segid 3A4 and resid 347 and name CA)	(segid 3A4 and resid 353 and name CA)	10.13	0.39	0.38
	assign (segid 3A4 and resid 347 and name CA)	(segid 3A4 and resid 353 and name CB)	9.68	0.31	0.32
	assign (segid 3A4 and resid 347 and name CA)	(segid 3A4 and resid 354 and name CA)	13.83	0.37	0.38
	assign (segid 3A4 and resid 347 and name CA)	(segid 3A4 and resid 354 and name CB)	14.81	0.46	0.45
	assign (segid 3A4 and resid 347 and name CA)	(segid 3A4 and resid 355 and name CA)	14.81	0.29	0.30
10	assign (segid 3A4 and resid 347 and name CA)	(segid 3A4 and resid 355 and name CB)	14.71	0.43	0.44
	assign (segid 3A4 and resid 347 and name CA)	(segid 3A4 and resid 356 and name CA)	13.16	0.27	0.26
	assign (segid 3A4 and resid 347 and name CA)	(segid 3A4 and resid 356 and name CB)	11.77	0.28	0.28
	assign (segid 3A4 and resid 347 and name CA)	(segid 3A4 and resid 357 and name CA)	13.65	0.37	0.37
	assign (segid 3A4 and resid 347 and name CA)	(segid 3A4 and resid 357 and name CB)	12.59	0.43	0.43
15	assign (segid 3A4 and resid 347 and name CA)	(segid 3A4 and resid 358 and name CA)	16.94	0.42	0.42
	assign (segid 3A4 and resid 347 and name CA)	(segid 3A4 and resid 358 and name CB)	18.26	0.44	0.45
	assign (segid 3A4 and resid 347 and name CA)	(segid 3A4 and resid 359 and name CA)	17.17	0.42	0.43
	assign (segid 3A4 and resid 347 and name CA)	(segid 3A4 and resid 359 and name CB)	18.37	0.42	0.42
	assign (segid 3A4 and resid 347 and name CA)	(segid 3A4 and resid 360 and name CA)	13.47	0.44	0.44
20	assign (segid 3A4 and resid 347 and name CA)	(segid 3A4 and resid 360 and name CB)	12.57	0.44	0.45
	assign (segid 3A4 and resid 347 and name CA)	(segid 3A4 and resid 361 and name CA)	14.58	0.47	0.47
	assign (segid 3A4 and resid 347 and name CA)	(segid 3A4 and resid 361 and name CB)	15.19	0.45	0.44
	assign (segid 3A4 and resid 347 and name CA)	(segid 3A4 and resid 362 and name CA)	17.14	0.47	0.46
	assign (segid 3A4 and resid 347 and name CA)	(segid 3A4 and resid 362 and name CB)	18.21	0.45	0.44
25	assign (segid 3A4 and resid 347 and name CA)	(segid 3A4 and resid 363 and name CA)	17.02	0.45	0.44
	assign (segid 3A4 and resid 347 and name CA)	(segid 3A4 and resid 363 and name CB)	17.37	0.34	0.34
	assign (segid 3A4 and resid 347 and name CA)	(segid 3A4 and resid 364 and name CA)	18.82	0.46	0.45
	assign (segid 3A4 and resid 347 and name CA)	(segid 3A4 and resid 381 and name CA)	8.41	0.33	0.34
	assign (segid 3A4 and resid 347 and name CA)	(segid 3A4 and resid 382 and name C)	5.53	0.49	0.49
30	assign (segid 3A4 and resid 347 and name CA)	(segid 3A4 and resid 382 and name CA)	6.00	0.49	0.49
	assign (segid 3A4 and resid 347 and name CA)	(segid 3A4 and resid 382 and name CB)	5.24	0.57	0.57
	assign (segid 3A4 and resid 347 and name CA)	(segid 3A4 and resid 382 and name N)	6.46	0.39	0.39
	assign (segid 3A4 and resid 347 and name CA)	(segid 3A4 and resid 382 and name O)	4.86	0.52	0.52
	assign (segid 3A4 and resid 347 and name CA)	(segid 3A4 and resid 383 and name C)	7.00	0.52	0.53
35	assign (segid 3A4 and resid 347 and name CA)	(segid 3A4 and resid 383 and name CA)	6.34	0.40	0.41
	assign (segid 3A4 and resid 347 and name CA)	(segid 3A4 and resid 383 and name N)	6.26	0.44	0.44
	assign (segid 3A4 and resid 347 and name CA)	(segid 3A4 and resid 383 and name O)	7.06	0.60	0.61
	assign (segid 3A4 and resid 347 and name CA)	(segid 3A4 and resid 384 and name CA)	8.73	0.58	0.59
	assign (segid 3A4 and resid 347 and name CA)	(segid 3A4 and resid 384 and name CB)	10.11	0.54	0.55
40	assign (segid 3A4 and resid 347 and name CA)	(segid 3A4 and resid 385 and name CA)	7.35	0.73	0.73
	assign (segid 3A4 and resid 347 and name CA)	(segid 3A4 and resid 386 and name CA)	9.66	0.74	0.74
	assign (segid 3A4 and resid 347 and name CA)	(segid 3A4 and resid 387 and name CA)	12.83	0.92	0.92
	assign (segid 3A4 and resid 347 and name CA)	(segid 3A4 and resid 388 and name CA)	15.49	0.90	0.90
	assign (segid 3A4 and resid 347 and name CA)	(segid 3A4 and resid 388 and name CB)	16.51	0.99	0.99
45	assign (segid 3A4 and resid 347 and name CA)	(segid 3A4 and resid 389 and name CA)	13.56	0.86	0.85
	assign (segid 3A4 and resid 347 and name CA)	(segid 3A4 and resid 389 and name CB)	13.03	0.90	0.91
	assign (segid 3A4 and resid 347 and name CA)	(segid 3A4 and resid 390 and name CA)	12.04	0.63	0.63
	assign (segid 3A4 and resid 347 and name CA)	(segid 3A4 and resid 390 and name CB)	12.49	0.56	0.57
	assign (segid 3A4 and resid 347 and name CA)	(segid 3A4 and resid 391 and name CA)	12.86	0.67	0.67
50	assign (segid 3A4 and resid 347 and name CA)	(segid 3A4 and resid 391 and name CB)	12.24	0.69	0.69
	assign (segid 3A4 and resid 347 and name CA)	(segid 3A4 and resid 392 and name CA)	16.63	0.67	0.67
	assign (segid 3A4 and resid 347 and name CA)	(segid 3A4 and resid 392 and name CB)	17.55	0.69	0.70
	assign (segid 3A4 and resid 347 and name CA)	(segid 3A4 and resid 393 and name CA)	17.05	0.70	0.69
	assign (segid 3A4 and resid 347 and name CA)	(segid 3A4 and resid 394 and name CA)	15.20	0.59	0.59
55	assign (segid 3A4 and resid 347 and name CA)	(segid 3A4 and resid 394 and name CB)	14.55	0.70	0.71
	assign (segid 3A4 and resid 347 and name CA)	(segid 3A4 and resid 395 and name CA)	18.67	0.59	0.59
	assign (segid 3A4 and resid 347 and name CA)	(segid 3A4 and resid 397 and name CA)	17.27	0.56	0.57
	assign (segid 3A4 and resid 347 and name CA)	(segid 3A4 and resid 397 and name CB)	15.83	0.59	0.59
	assign (segid 3A4 and resid 347 and name CA)	(segid 3A4 and resid 398 and name C)	17.74	0.41	0.41
60	assign (segid 3A4 and resid 347 and name CA)	(segid 3A4 and resid 398 and name CB)	17.50	0.43	0.43
	assign (segid 3A4 and resid 347 and name CA)	(segid 3A4 and resid 427 and name CA)	16.90	0.83	0.83
	assign (segid 3A4 and resid 347 and name CA)	(segid 3A4 and resid 428 and name CA)	16.50	1.24	1.24
	assign (segid 3A4 and resid 347 and name CA)	(segid 3A4 and resid 429 and name CA)	14.81	1.17	1.18
	assign (segid 3A4 and resid 347 and name CA)	(segid 3A4 and resid 430 and name CA)	13.35	1.88	1.87
65	assign (segid 3A4 and resid 347 and name CA)	(segid 3A4 and resid 431 and name CA)	11.82	1.46	1.45
	assign (segid 3A4 and resid 347 and name CA)	(segid 3A4 and resid 433 and name CA)	12.13	0.39	0.38
	assign (segid 3A4 and resid 347 and name CA)	(segid 3A4 and resid 434 and name CA)	14.87	0.95	0.95
	assign (segid 3A4 and resid 347 and name CA)	(segid 3A4 and resid 435 and name CA)	17.94	0.81	0.81
	assign (segid 3A4 and resid 347 and name CB)	(segid 3A4 and resid 348 and name C)	5.46	0.11	0.11
70	assign (segid 3A4 and resid 347 and name CB)	(segid 3A4 and resid 348 and name CA)	4.55	0.09	0.08
	assign (segid 3A4 and resid 347 and name CB)	(segid 3A4 and resid 348 and name N)	3.22	0.07	0.08
	assign (segid 3A4 and resid 347 and name CB)	(segid 3A4 and resid 348 and name O)	6.34	0.14	0.13
	assign (segid 3A4 and resid 347 and name CB)	(segid 3A4 and resid 349 and name C)	6.86	0.18	0.18
	assign (segid 3A4 and resid 347 and name CB)	(segid 3A4 and resid 349 and name CA)	6.82	0.16	0.16
75	assign (segid 3A4 and resid 347 and name CB)	(segid 3A4 and resid 349 and name CB)	7.35	0.21	0.20
	assign (segid 3A4 and resid 347 and name CB)	(segid 3A4 and resid 349 and name N)	5.66	0.15	0.14
	assign (segid 3A4 and resid 347 and name CB)	(segid 3A4 and resid 350 and name CA)	6.41	0.35	0.35
	assign (segid 3A4 and resid 347 and name CB)	(segid 3A4 and resid 350 and name CB)	5.64	0.43	0.43
	assign (segid 3A4 and resid 347 and name CB)	(segid 3A4 and resid 350 and name N)	5.96	0.26	0.26
80	assign (segid 3A4 and resid 347 and name CB)	(segid 3A4 and resid 351 and name CA)	7.15	0.71	0.71
	assign (segid 3A4 and resid 347 and name CB)	(segid 3A4 and resid 351 and name N)	6.32	0.59	0.59
	assign (segid 3A4 and resid 347 and name CB)	(segid 3A4 and resid 352 and name CA)	9.88	0.45	0.44
	assign (segid 3A4 and resid 347 and name CB)	(segid 3A4 and resid 352 and name CB)	9.94	0.37	0.37

	assign (segid 3A4 and resid 347 and name CB) (segid 3A4 and resid 353 and name CA)	11.35	0.44	0.44
	assign (segid 3A4 and resid 347 and name CB) (segid 3A4 and resid 353 and name CB)	10.91	0.38	0.38
	assign (segid 3A4 and resid 347 and name CB) (segid 3A4 and resid 354 and name CA)	15.00	0.42	0.42
	assign (segid 3A4 and resid 347 and name CB) (segid 3A4 and resid 354 and name CB)	16.03	0.51	0.50
5	assign (segid 3A4 and resid 347 and name CB) (segid 3A4 and resid 355 and name CA)	15.95	0.33	0.34
	assign (segid 3A4 and resid 347 and name CB) (segid 3A4 and resid 355 and name CB)	15.90	0.46	0.47
	assign (segid 3A4 and resid 347 and name CB) (segid 3A4 and resid 356 and name CA)	14.04	0.30	0.29
	assign (segid 3A4 and resid 347 and name CB) (segid 3A4 and resid 356 and name CB)	12.62	0.30	0.30
	assign (segid 3A4 and resid 347 and name CB) (segid 3A4 and resid 357 and name CA)	14.40	0.43	0.43
10	assign (segid 3A4 and resid 347 and name CB) (segid 3A4 and resid 357 and name CB)	13.29	0.48	0.48
	assign (segid 3A4 and resid 347 and name CB) (segid 3A4 and resid 358 and name CA)	17.81	0.50	0.49
	assign (segid 3A4 and resid 347 and name CB) (segid 3A4 and resid 359 and name CA)	17.99	0.48	0.49
	assign (segid 3A4 and resid 347 and name CB) (segid 3A4 and resid 360 and name CA)	14.25	0.50	0.51
	assign (segid 3A4 and resid 347 and name CB) (segid 3A4 and resid 360 and name CB)	13.47	0.50	0.50
15	assign (segid 3A4 and resid 347 and name CB) (segid 3A4 and resid 361 and name CA)	15.27	0.53	0.54
	assign (segid 3A4 and resid 347 and name CB) (segid 3A4 and resid 361 and name CB)	15.96	0.50	0.50
	assign (segid 3A4 and resid 347 and name CB) (segid 3A4 and resid 362 and name CA)	17.61	0.54	0.54
	assign (segid 3A4 and resid 347 and name CB) (segid 3A4 and resid 363 and name CA)	17.16	0.51	0.51
	assign (segid 3A4 and resid 347 and name CB) (segid 3A4 and resid 363 and name CB)	17.43	0.38	0.38
20	assign (segid 3A4 and resid 347 and name CB) (segid 3A4 and resid 381 and name CA)	8.29	0.29	0.28
	assign (segid 3A4 and resid 347 and name CB) (segid 3A4 and resid 382 and name C)	4.71	0.41	0.41
	assign (segid 3A4 and resid 347 and name CB) (segid 3A4 and resid 382 and name CB)	5.49	0.46	0.46
	assign (segid 3A4 and resid 347 and name CB) (segid 3A4 and resid 382 and name N)	4.97	0.57	0.56
25	assign (segid 3A4 and resid 347 and name CB) (segid 3A4 and resid 382 and name O)	6.16	0.34	0.34
	assign (segid 3A4 and resid 347 and name CB) (segid 3A4 and resid 383 and name C)	3.87	0.46	0.45
	assign (segid 3A4 and resid 347 and name CB) (segid 3A4 and resid 383 and name CB)	5.72	0.45	0.44
	assign (segid 3A4 and resid 347 and name CB) (segid 3A4 and resid 383 and name CA)	5.25	0.28	0.28
	assign (segid 3A4 and resid 347 and name CB) (segid 3A4 and resid 383 and name N)	5.38	0.34	0.33
30	assign (segid 3A4 and resid 347 and name CB) (segid 3A4 and resid 383 and name O)	5.66	0.55	0.55
	assign (segid 3A4 and resid 347 and name CB) (segid 3A4 and resid 384 and name CA)	7.39	0.56	0.56
	assign (segid 3A4 and resid 347 and name CB) (segid 3A4 and resid 384 and name CB)	8.81	0.52	0.53
	assign (segid 3A4 and resid 347 and name CB) (segid 3A4 and resid 384 and name N)	6.55	0.47	0.46
	assign (segid 3A4 and resid 347 and name CB) (segid 3A4 and resid 385 and name CA)	6.24	0.72	0.72
	assign (segid 3A4 and resid 347 and name CB) (segid 3A4 and resid 385 and name N)	6.10	0.66	0.66
35	assign (segid 3A4 and resid 347 and name CB) (segid 3A4 and resid 386 and name CA)	8.98	0.72	0.72
	assign (segid 3A4 and resid 347 and name CB) (segid 3A4 and resid 387 and name CA)	12.20	0.87	0.86
	assign (segid 3A4 and resid 347 and name CB) (segid 3A4 and resid 388 and name CA)	14.66	0.87	0.86
	assign (segid 3A4 and resid 347 and name CB) (segid 3A4 and resid 388 and name CB)	15.72	0.94	0.95
	assign (segid 3A4 and resid 347 and name CB) (segid 3A4 and resid 389 and name CA)	12.51	0.87	0.87
40	assign (segid 3A4 and resid 347 and name CB) (segid 3A4 and resid 389 and name CB)	12.04	0.93	0.92
	assign (segid 3A4 and resid 347 and name CB) (segid 3A4 and resid 390 and name CA)	10.88	0.63	0.63
	assign (segid 3A4 and resid 347 and name CB) (segid 3A4 and resid 390 and name CB)	11.40	0.57	0.58
	assign (segid 3A4 and resid 347 and name CB) (segid 3A4 and resid 391 and name CA)	11.45	0.66	0.67
45	assign (segid 3A4 and resid 347 and name CB) (segid 3A4 and resid 391 and name CB)	10.80	0.69	0.68
	assign (segid 3A4 and resid 347 and name CB) (segid 3A4 and resid 392 and name CA)	15.21	0.66	0.67
	assign (segid 3A4 and resid 347 and name CB) (segid 3A4 and resid 392 and name CB)	16.13	0.69	0.69
	assign (segid 3A4 and resid 347 and name CB) (segid 3A4 and resid 393 and name CA)	15.56	0.68	0.69
	assign (segid 3A4 and resid 347 and name CB) (segid 3A4 and resid 394 and name CA)	13.81	0.57	0.58
50	assign (segid 3A4 and resid 347 and name CB) (segid 3A4 and resid 394 and name CB)	13.22	0.70	0.70
	assign (segid 3A4 and resid 347 and name CB) (segid 3A4 and resid 395 and name CA)	17.34	0.58	0.57
	assign (segid 3A4 and resid 347 and name CB) (segid 3A4 and resid 396 and name CA)	18.64	0.60	0.59
	assign (segid 3A4 and resid 347 and name CB) (segid 3A4 and resid 397 and name CA)	15.89	0.52	0.52
	assign (segid 3A4 and resid 347 and name CB) (segid 3A4 and resid 397 and name CB)	14.43	0.55	0.54
	assign (segid 3A4 and resid 347 and name CB) (segid 3A4 and resid 398 and name CA)	16.51	0.37	0.37
55	assign (segid 3A4 and resid 347 and name CB) (segid 3A4 and resid 398 and name CB)	16.32	0.41	0.40
	assign (segid 3A4 and resid 347 and name CB) (segid 3A4 and resid 401 and name CA)	18.56	0.29	0.29
	assign (segid 3A4 and resid 347 and name CB) (segid 3A4 and resid 427 and name CA)	16.62	0.94	0.93
	assign (segid 3A4 and resid 347 and name CB) (segid 3A4 and resid 428 and name CA)	16.28	1.39	1.40
60	assign (segid 3A4 and resid 347 and name CB) (segid 3A4 and resid 429 and name CA)	14.57	1.29	1.29
	assign (segid 3A4 and resid 347 and name CB) (segid 3A4 and resid 430 and name CA)	13.09	1.89	1.89
	assign (segid 3A4 and resid 347 and name CB) (segid 3A4 and resid 431 and name CA)	11.23	1.58	1.58
	assign (segid 3A4 and resid 347 and name CB) (segid 3A4 and resid 433 and name CA)	11.57	0.49	0.49
	assign (segid 3A4 and resid 347 and name CB) (segid 3A4 and resid 434 and name CA)	14.23	0.97	0.98
65	assign (segid 3A4 and resid 347 and name CB) (segid 3A4 and resid 435 and name CA)	17.39	0.90	0.91
	assign (segid 3A4 and resid 347 and name CB) (segid HEM and resid 1 and name CMA)	5.92	0.74	0.75
	assign (segid 3A4 and resid 347 and name N) (segid 3A4 and resid 347 and name C)	2.45	0.02	0.02
	assign (segid 3A4 and resid 347 and name N) (segid 3A4 and resid 347 and name CA)	1.45	0.01	0.01
	assign (segid 3A4 and resid 347 and name N) (segid 3A4 and resid 347 and name CB)	2.46	0.01	0.01
	assign (segid 3A4 and resid 347 and name N) (segid 3A4 and resid 347 and name O)	3.49	0.05	0.06
70	assign (segid 3A4 and resid 347 and name N) (segid 3A4 and resid 348 and name C)	4.75	0.11	0.11
	assign (segid 3A4 and resid 347 and name N) (segid 3A4 and resid 348 and name CA)	4.21	0.11	0.11
	assign (segid 3A4 and resid 347 and name N) (segid 3A4 and resid 348 and name N)	2.80	0.13	0.12
	assign (segid 3A4 and resid 347 and name N) (segid 3A4 and resid 348 and name O)	5.87	0.12	0.13
	assign (segid 3A4 and resid 347 and name N) (segid 3A4 and resid 349 and name C)	5.73	0.16	0.16
75	assign (segid 3A4 and resid 347 and name N) (segid 3A4 and resid 349 and name CA)	5.42	0.16	0.15
	assign (segid 3A4 and resid 347 and name N) (segid 3A4 and resid 349 and name CB)	5.52	0.21	0.20
	assign (segid 3A4 and resid 347 and name N) (segid 3A4 and resid 349 and name N)	4.38	0.14	0.15
	assign (segid 3A4 and resid 347 and name N) (segid 3A4 and resid 349 and name O)	6.94	0.19	0.18
	assign (segid 3A4 and resid 347 and name N) (segid 3A4 and resid 350 and name C)	6.72	0.45	0.45
80	assign (segid 3A4 and resid 347 and name N) (segid 3A4 and resid 350 and name CA)	5.79	0.36	0.36
	assign (segid 3A4 and resid 347 and name N) (segid 3A4 and resid 350 and name CB)	5.27	0.52	0.52
	assign (segid 3A4 and resid 347 and name N) (segid 3A4 and resid 350 and name N)	4.99	0.28	0.28
	assign (segid 3A4 and resid 347 and name N) (segid 3A4 and resid 351 and name N)	6.41	0.50	0.50

5	assign	(segid 3A4 and resid 347 and name N)	(segid 3A4 and resid 382 and name C)	6.83	0.43	0.43
	assign	(segid 3A4 and resid 347 and name N)	(segid 3A4 and resid 382 and name CB)	6.44	0.50	0.49
	assign	(segid 3A4 and resid 347 and name N)	(segid 3A4 and resid 382 and name O)	6.05	0.45	0.45
	assign	(segid 3A4 and resid 347 and name O)	(segid 3A4 and resid 347 and name CB)	3.25	0.04	0.05
10	assign	(segid 3A4 and resid 347 and name O)	(segid 3A4 and resid 348 and name C)	2.93	0.13	0.12
	assign	(segid 3A4 and resid 347 and name O)	(segid 3A4 and resid 348 and name CA)	2.76	0.05	0.05
	assign	(segid 3A4 and resid 347 and name O)	(segid 3A4 and resid 348 and name N)	2.24	0.04	0.04
	assign	(segid 3A4 and resid 347 and name O)	(segid 3A4 and resid 348 and name O)	3.47	0.18	0.17
15	assign	(segid 3A4 and resid 347 and name O)	(segid 3A4 and resid 349 and name C)	4.03	0.19	0.20
	assign	(segid 3A4 and resid 347 and name O)	(segid 3A4 and resid 349 and name CA)	4.28	0.20	0.20
	assign	(segid 3A4 and resid 347 and name O)	(segid 3A4 and resid 349 and name CB)	5.27	0.21	0.21
	assign	(segid 3A4 and resid 347 and name O)	(segid 3A4 and resid 349 and name N)	3.34	0.17	0.17
20	assign	(segid 3A4 and resid 347 and name O)	(segid 3A4 and resid 349 and name O)	4.99	0.21	0.21
	assign	(segid 3A4 and resid 347 and name O)	(segid 3A4 and resid 350 and name C)	4.01	0.42	0.41
	assign	(segid 3A4 and resid 347 and name O)	(segid 3A4 and resid 350 and name CA)	3.79	0.23	0.23
	assign	(segid 3A4 and resid 347 and name O)	(segid 3A4 and resid 350 and name CB)	3.64	0.17	0.17
25	assign	(segid 3A4 and resid 347 and name O)	(segid 3A4 and resid 350 and name N)	3.26	0.22	0.23
	assign	(segid 3A4 and resid 347 and name O)	(segid 3A4 and resid 350 and name O)	5.17	0.41	0.42
	assign	(segid 3A4 and resid 347 and name O)	(segid 3A4 and resid 351 and name C)	5.30	0.53	0.53
	assign	(segid 3A4 and resid 347 and name O)	(segid 3A4 and resid 351 and name CA)	4.20	0.60	0.59
30	assign	(segid 3A4 and resid 347 and name O)	(segid 3A4 and resid 351 and name N)	3.26	0.50	0.50
	assign	(segid 3A4 and resid 347 and name O)	(segid 3A4 and resid 351 and name O)	6.35	0.56	0.57
	assign	(segid 3A4 and resid 347 and name O)	(segid 3A4 and resid 352 and name CA)	6.68	0.43	0.42
	assign	(segid 3A4 and resid 347 and name O)	(segid 3A4 and resid 352 and name CB)	6.83	0.35	0.35
35	assign	(segid 3A4 and resid 347 and name O)	(segid 3A4 and resid 352 and name CG)	6.69	0.21	0.21
	assign	(segid 3A4 and resid 347 and name O)	(segid 3A4 and resid 352 and name N)	5.37	0.47	0.46
	assign	(segid 3A4 and resid 347 and name O)	(segid 3A4 and resid 381 and name C)	6.83	0.64	0.63
	assign	(segid 3A4 and resid 347 and name O)	(segid 3A4 and resid 382 and name C)	5.45	0.77	0.77
40	assign	(segid 3A4 and resid 347 and name O)	(segid 3A4 and resid 382 and name CA)	5.73	0.75	0.74
	assign	(segid 3A4 and resid 347 and name O)	(segid 3A4 and resid 382 and name CB)	5.26	0.77	0.77
	assign	(segid 3A4 and resid 347 and name O)	(segid 3A4 and resid 382 and name N)	5.64	0.66	0.66
	assign	(segid 3A4 and resid 347 and name O)	(segid 3A4 and resid 382 and name O)	5.29	0.75	0.74
45	assign	(segid 3A4 and resid 347 and name O)	(segid 3A4 and resid 383 and name CA)	6.16	0.68	0.67
	assign	(segid 3A4 and resid 347 and name O)	(segid 3A4 and resid 383 and name N)	5.90	0.74	0.73
	assign	(segid 3A4 and resid 348 and name C)	(segid 3A4 and resid 348 and name O)	1.24	0.01	0.01
	assign	(segid 3A4 and resid 348 and name C)	(segid 3A4 and resid 349 and name C)	3.09	0.06	0.05
50	assign	(segid 3A4 and resid 348 and name C)	(segid 3A4 and resid 349 and name CA)	2.44	0.02	0.03
	assign	(segid 3A4 and resid 348 and name C)	(segid 3A4 and resid 349 and name CB)	3.71	0.02	0.01
	assign	(segid 3A4 and resid 348 and name C)	(segid 3A4 and resid 349 and name N)	1.34	0.01	0.01
	assign	(segid 3A4 and resid 348 and name C)	(segid 3A4 and resid 349 and name O)	3.95	0.10	0.10
55	assign	(segid 3A4 and resid 348 and name C)	(segid 3A4 and resid 350 and name C)	4.73	0.20	0.19
	assign	(segid 3A4 and resid 348 and name C)	(segid 3A4 and resid 350 and name CA)	4.57	0.11	0.11
	assign	(segid 3A4 and resid 348 and name C)	(segid 3A4 and resid 350 and name CB)	5.28	0.08	0.08
	assign	(segid 3A4 and resid 348 and name C)	(segid 3A4 and resid 350 and name N)	3.37	0.11	0.11
60	assign	(segid 3A4 and resid 348 and name C)	(segid 3A4 and resid 350 and name O)	5.82	0.22	0.22
	assign	(segid 3A4 and resid 348 and name C)	(segid 3A4 and resid 351 and name C)	5.08	0.30	0.29
	assign	(segid 3A4 and resid 348 and name C)	(segid 3A4 and resid 351 and name CA)	4.78	0.32	0.32
	assign	(segid 3A4 and resid 348 and name C)	(segid 3A4 and resid 351 and name N)	4.01	0.23	0.24
65	assign	(segid 3A4 and resid 348 and name C)	(segid 3A4 and resid 351 and name O)	6.11	0.33	0.34
	assign	(segid 3A4 and resid 348 and name C)	(segid 3A4 and resid 352 and name C)	6.30	0.36	0.36
	assign	(segid 3A				

assign (segid 3A4 and resid 348 and name CA) (segid 3A4 and resid 356 and name CB) 11.79 0.33 0.33
assign (segid 3A4 and resid 348 and name CA) (segid 3A4 and resid 357 and name CA) 12.48 0.23 0.24
assign (segid 3A4 and resid 348 and name CA) (segid 3A4 and resid 357 and name CB) 11.25 0.28 0.28
assign (segid 3A4 and resid 348 and name CA) (segid 3A4 and resid 358 and name CA) 15.16 0.35 0.35
5 assign (segid 3A4 and resid 348 and name CA) (segid 3A4 and resid 358 and name CB) 16.54 0.37 0.38
assign (segid 3A4 and resid 348 and name CA) (segid 3A4 and resid 359 and name CA) 14.69 0.46 0.45
assign (segid 3A4 and resid 348 and name CA) (segid 3A4 and resid 359 and name CB) 15.84 0.48 0.47
assign (segid 3A4 and resid 348 and name CA) (segid 3A4 and resid 360 and name CA) 10.92 0.43 0.43
assign (segid 3A4 and resid 348 and name CA) (segid 3A4 and resid 360 and name CB) 10.13 0.44 0.44
10 assign (segid 3A4 and resid 348 and name CA) (segid 3A4 and resid 361 and name CA) 11.32 0.50 0.50
assign (segid 3A4 and resid 348 and name CA) (segid 3A4 and resid 361 and name CB) 11.81 0.49 0.50
assign (segid 3A4 and resid 348 and name CA) (segid 3A4 and resid 362 and name CA) 14.08 0.45 0.46
assign (segid 3A4 and resid 348 and name CA) (segid 3A4 and resid 362 and name CB) 15.27 0.43 0.43
assign (segid 3A4 and resid 348 and name CA) (segid 3A4 and resid 363 and name CA) 14.19 0.39 0.39
15 assign (segid 3A4 and resid 348 and name CA) (segid 3A4 and resid 363 and name CB) 14.46 0.31 0.32
assign (segid 3A4 and resid 348 and name CA) (segid 3A4 and resid 364 and name CA) 16.50 0.40 0.40
assign (segid 3A4 and resid 348 and name CA) (segid 3A4 and resid 364 and name CB) 16.80 0.41 0.42
assign (segid 3A4 and resid 348 and name CA) (segid 3A4 and resid 365 and name CA) 17.54 0.48 0.47
20 assign (segid 3A4 and resid 348 and name CA) (segid 3A4 and resid 365 and name CB) 18.48 0.45 0.46
assign (segid 3A4 and resid 348 and name CA) (segid 3A4 and resid 381 and name CA) 9.28 0.60 0.61
assign (segid 3A4 and resid 348 and name CA) (segid 3A4 and resid 382 and name CA) 8.17 0.68 0.68
assign (segid 3A4 and resid 348 and name CA) (segid 3A4 and resid 382 and name CB) 7.88 0.70 0.70
assign (segid 3A4 and resid 348 and name CA) (segid 3A4 and resid 383 and name CA) 7.53 0.73 0.73
25 assign (segid 3A4 and resid 348 and name CA) (segid 3A4 and resid 384 and name CA) 10.83 0.77 0.77
assign (segid 3A4 and resid 348 and name CA) (segid 3A4 and resid 384 and name CB) 12.10 0.74 0.75
assign (segid 3A4 and resid 348 and name CA) (segid 3A4 and resid 385 and name CA) 10.53 0.79 0.79
assign (segid 3A4 and resid 348 and name CA) (segid 3A4 and resid 386 and name CA) 13.11 0.82 0.81
30 assign (segid 3A4 and resid 348 and name CA) (segid 3A4 and resid 387 and name CA) 16.45 0.91 0.92
assign (segid 3A4 and resid 348 and name CA) (segid 3A4 and resid 389 and name CA) 17.02 0.90 0.90
assign (segid 3A4 and resid 348 and name CA) (segid 3A4 and resid 389 and name CB) 16.53 0.96 0.96
assign (segid 3A4 and resid 348 and name CA) (segid 3A4 and resid 390 and name CA) 15.20 0.69 0.69
assign (segid 3A4 and resid 348 and name CA) (segid 3A4 and resid 390 and name CB) 15.62 0.60 0.60
35 assign (segid 3A4 and resid 348 and name CA) (segid 3A4 and resid 391 and name CA) 15.39 0.76 0.76
assign (segid 3A4 and resid 348 and name CA) (segid 3A4 and resid 391 and name CB) 14.49 0.81 0.81
assign (segid 3A4 and resid 348 and name CA) (segid 3A4 and resid 394 and name CA) 16.80 0.76 0.77
assign (segid 3A4 and resid 348 and name CA) (segid 3A4 and resid 394 and name CB) 16.34 0.86 0.87
40 assign (segid 3A4 and resid 348 and name CA) (segid 3A4 and resid 397 and name CA) 17.91 0.86 0.86
assign (segid 3A4 and resid 348 and name CA) (segid 3A4 and resid 397 and name CB) 16.55 0.88 0.88
assign (segid 3A4 and resid 348 and name CA) (segid 3A4 and resid 398 and name CA) 18.14 0.66 0.65
45 assign (segid 3A4 and resid 348 and name CA) (segid 3A4 and resid 398 and name CB) 18.06 0.63 0.64
assign (segid 3A4 and resid 348 and name CA) (segid 3A4 and resid 426 and name CA) 15.38 1.44 1.45
assign (segid 3A4 and resid 348 and name CA) (segid 3A4 and resid 427 and name CA) 14.40 0.77 0.76
50 assign (segid 3A4 and resid 348 and name CA) (segid 3A4 and resid 428 and name CA) 14.36 1.03 1.03
assign (segid 3A4 and resid 348 and name CA) (segid 3A4 and resid 429 and name CA) 13.20 1.01 1.00
55 assign (segid 3A4 and resid 348 and name CA) (segid 3A4 and resid 430 and name CA) 12.43 1.75 1.75
assign (segid 3A4 and resid 348 and name CA) (segid 3A4 and resid 431 and name CA) 11.69 1.13 1.14
assign (segid 3A4 and resid 348 and name CA) (segid 3A4 and resid 433 and name CA) 10.32 0.47 0.47
assign (segid 3A4 and resid 348 and name CA) (segid 3A4 and resid 434 and name CA) 12.78 0.95 0.95
60 assign (segid 3A4 and resid 348 and name CA) (segid 3A4 and resid 435 and name CA) 15.46 0.69 0.70
assign (segid 3A4 and resid 348 and name N) (segid 3A4 and resid 348 and name C) 2.48 0.06 0.05
assign (segid 3A4 and resid 348 and name N) (segid 3A4 and resid 348 and name CA) 1.46 0.01 0.02
assign (segid 3A4 and resid 348 and name N) (segid 3A4 and resid 348 and name O) 3.54 0.07 0.06
assign (segid 3A4 and resid 348 and name N) (segid 3A4 and resid 349 and name C) 4.75 0.10 0.11
65 assign (segid 3A4 and resid 348 and name N) (segid 3A4 and resid 349 and name CA) 4.24 0.10 0.11
assign (segid 3A4 and resid 348 and name N) (segid 3A4 and resid 349 and name CB) 5.00 0.11 0.12
assign (segid 3A4 and resid 348 and name N) (segid 3A4 and resid 349 and name N) 2.84 0.11 0.11
assign (segid 3A4 and resid 348 and name N) (segid 3A4 and resid 349 and name O) 5.85 0.14 0.14
70 assign (segid 3A4 and resid 348 and name N) (segid 3A4 and resid 350 and name C) 5.84 0.37 0.36
assign (segid 3A4 and resid 348 and name N) (segid 3A4 and resid 350 and name CA) 5.43 0.23 0.23
assign (segid 3A4 and resid 348 and name N) (segid 3A4 and resid 350 and name CB) 5.46 0.28 0.28
assign (segid 3A4 and resid 348 and name N) (segid 3A4 and resid 350 and name N) 4.40 0.18 0.18
75 assign (segid 3A4 and resid 348 and name N) (segid 3A4 and resid 350 and name O) 7.04 0.36 0.35
assign (segid 3A4 and resid 348 and name N) (segid 3A4 and resid 351 and name C) 6.72 0.48 0.48
assign (segid 3A4 and resid 348 and name N) (segid 3A4 and resid 351 and name CA) 5.93 0.56 0.55
80 assign (segid 3A4 and resid 348 and name N) (segid 3A4 and resid 351 and name N) 5.09 0.45 0.45
assign (segid 3A4 and resid 348 and name N) (segid 3A4 and resid 352 and name CB) 7.31 0.33 0.33
assign (segid 3A4 and resid 348 and name N) (segid 3A4 and resid 352 and name CG) 6.95 0.18 0.19
assign (segid 3A4 and resid 348 and name N) (segid 3A4 and resid 352 and name N) 6.54 0.41 0.41
assign (segid 3A4 and resid 348 and name N) (segid 3A4 and resid 382 and name O) 6.41 0.66 0.65
70 assign (segid 3A4 and resid 348 and name N) (segid 3A4 and resid 383 and name CA) 7.01 0.62 0.63
assign (segid 3A4 and resid 348 and name O) (segid 3A4 and resid 349 and name C) 3.08 0.09 0.10
assign (segid 3A4 and resid 348 and name O) (segid 3A4 and resid 349 and name CA) 2.77 0.03 0.02
assign (segid 3A4 and resid 348 and name O) (segid 3A4 and resid 349 and name CB) 4.23 0.03 0.02
75 assign (segid 3A4 and resid 348 and name O) (segid 3A4 and resid 349 and name N) 2.25 0.01 0.01
assign (segid 3A4 and resid 348 and name O) (segid 3A4 and resid 349 and name O) 3.59 0.10 0.10
80 assign (segid 3A4 and resid 348 and name O) (segid 3A4 and resid 350 and name C) 4.35 0.22 0.22
assign (segid 3A4 and resid 348 and name O) (segid 3A4 and resid 350 and name CA) 4.55 0.18 0.18
assign (segid 3A4 and resid 348 and name O) (segid 3A4 and resid 350 and name CB) 5.47 0.10 0.10
assign (segid 3A4 and resid 348 and name O) (segid 3A4 and resid 350 and name N) 3.56 0.18 0.18
assign (segid 3A4 and resid 348 and name O) (segid 3A4 and resid 350 and name O) 5.30 0.28 0.28
assign (segid 3A4 and resid 348 and name O) (segid 3A4 and resid 351 and name C) 4.07 0.28 0.28
assign (segid 3A4 and resid 348 and name O) (segid 3A4 and resid 351 and name CA) 4.05 0.26 0.25
assign (segid 3A4 and resid 348 and name O) (segid 3A4 and resid 351 and name N) 3.55 0.17 0.18

	assign (segid 3A4 and resid 348 and name O)	(segid 3A4 and resid 351 and name O)	5.04	0.30	0.31
	assign (segid 3A4 and resid 348 and name O)	(segid 3A4 and resid 352 and name C)	5.32	0.43	0.44
	assign (segid 3A4 and resid 348 and name O)	(segid 3A4 and resid 352 and name CA)	4.30	0.32	0.32
	assign (segid 3A4 and resid 348 and name O)	(segid 3A4 and resid 352 and name CB)	3.86	0.24	0.25
5	assign (segid 3A4 and resid 348 and name O)	(segid 3A4 and resid 352 and name CG)	3.61	0.11	0.10
	assign (segid 3A4 and resid 348 and name O)	(segid 3A4 and resid 352 and name N)	3.52	0.32	0.32
	assign (segid 3A4 and resid 348 and name O)	(segid 3A4 and resid 352 and name O)	6.12	0.47	0.47
	assign (segid 3A4 and resid 348 and name O)	(segid 3A4 and resid 353 and name CA)	6.89	0.48	0.47
	assign (segid 3A4 and resid 348 and name O)	(segid 3A4 and resid 353 and name CB)	7.26	0.42	0.42
10	assign (segid 3A4 and resid 348 and name O)	(segid 3A4 and resid 353 and name N)	5.65	0.43	0.44
	assign (segid 3A4 and resid 349 and name C)	(segid 3A4 and resid 349 and name CB)	2.46	0.04	0.04
	assign (segid 3A4 and resid 349 and name C)	(segid 3A4 and resid 349 and name O)	1.24	0.03	0.02
	assign (segid 3A4 and resid 349 and name C)	(segid 3A4 and resid 350 and name C)	3.05	0.07	0.06
	assign (segid 3A4 and resid 349 and name C)	(segid 3A4 and resid 350 and name CA)	2.44	0.01	0.01
15	assign (segid 3A4 and resid 349 and name C)	(segid 3A4 and resid 350 and name CB)	3.72	0.03	0.02
	assign (segid 3A4 and resid 349 and name C)	(segid 3A4 and resid 350 and name N)	1.32	0.01	0.02
	assign (segid 3A4 and resid 349 and name C)	(segid 3A4 and resid 350 and name O)	3.93	0.05	0.05
	assign (segid 3A4 and resid 349 and name C)	(segid 3A4 and resid 351 and name C)	4.64	0.14	0.14
	assign (segid 3A4 and resid 349 and name C)	(segid 3A4 and resid 351 and name CA)	4.50	0.14	0.14
20	assign (segid 3A4 and resid 349 and name C)	(segid 3A4 and resid 351 and name N)	3.30	0.13	0.13
	assign (segid 3A4 and resid 349 and name C)	(segid 3A4 and resid 351 and name O)	5.83	0.13	0.13
	assign (segid 3A4 and resid 349 and name C)	(segid 3A4 and resid 352 and name C)	4.74	0.07	0.08
	assign (segid 3A4 and resid 349 and name C)	(segid 3A4 and resid 352 and name CA)	4.58	0.14	0.15
	assign (segid 3A4 and resid 349 and name C)	(segid 3A4 and resid 352 and name CB)	4.64	0.27	0.27
25	assign (segid 3A4 and resid 349 and name C)	(segid 3A4 and resid 352 and name CG)	5.31	0.41	0.41
	assign (segid 3A4 and resid 349 and name C)	(segid 3A4 and resid 352 and name N)	3.80	0.16	0.15
	assign (segid 3A4 and resid 349 and name C)	(segid 3A4 and resid 352 and name O)	5.52	0.15	0.15
	assign (segid 3A4 and resid 349 and name C)	(segid 3A4 and resid 353 and name C)	6.67	0.16	0.15
	assign (segid 3A4 and resid 349 and name C)	(segid 3A4 and resid 353 and name CA)	5.23	0.17	0.17
30	assign (segid 3A4 and resid 349 and name C)	(segid 3A4 and resid 353 and name CB)	5.17	0.24	0.23
	assign (segid 3A4 and resid 349 and name C)	(segid 3A4 and resid 353 and name CG)	6.20	0.25	0.25
	assign (segid 3A4 and resid 349 and name C)	(segid 3A4 and resid 353 and name N)	4.49	0.10	0.09
	assign (segid 3A4 and resid 349 and name C)	(segid 3A4 and resid 353 and name O)	7.25	0.17	0.17
	assign (segid 3A4 and resid 349 and name C)	(segid 3A4 and resid 353 and name OD1)	7.17	0.22	0.23
35	assign (segid 3A4 and resid 349 and name C)	(segid 3A4 and resid 354 and name N)	7.47	0.18	0.19
	assign (segid 3A4 and resid 349 and name CA)	(segid 3A4 and resid 349 and name C)	1.51	0.02	0.02
	assign (segid 3A4 and resid 349 and name CA)	(segid 3A4 and resid 349 and name CB)	1.51	0.02	0.02
	assign (segid 3A4 and resid 349 and name CA)	(segid 3A4 and resid 349 and name O)	2.37	0.03	0.02
40	assign (segid 3A4 and resid 349 and name CA)	(segid 3A4 and resid 350 and name C)	4.43	0.07	0.06
	assign (segid 3A4 and resid 349 and name CA)	(segid 3A4 and resid 350 and name CA)	3.81	0.02	0.03
	assign (segid 3A4 and resid 349 and name CA)	(segid 3A4 and resid 350 and name CB)	4.88	0.05	0.05
	assign (segid 3A4 and resid 349 and name CA)	(segid 3A4 and resid 350 and name N)	2.45	0.03	0.03
	assign (segid 3A4 and resid 349 and name CA)	(segid 3A4 and resid 350 and name O)	5.37	0.06	0.06
45	assign (segid 3A4 and resid 349 and name CA)	(segid 3A4 and resid 351 and name C)	5.54	0.13	0.13
	assign (segid 3A4 and resid 349 and name CA)	(segid 3A4 and resid 351 and name CA)	5.48	0.13	0.14
	assign (segid 3A4 and resid 349 and name CA)	(segid 3A4 and resid 351 and name N)	4.40	0.12	0.11
	assign (segid 3A4 and resid 349 and name CA)	(segid 3A4 and resid 351 and name O)	6.68	0.15	0.15
	assign (segid 3A4 and resid 349 and name CA)	(segid 3A4 and resid 352 and name C)	5.53	0.07	0.07
	assign (segid 3A4 and resid 349 and name CA)	(segid 3A4 and resid 352 and name CA)	5.21	0.12	0.13
50	assign (segid 3A4 and resid 349 and name CA)	(segid 3A4 and resid 352 and name CB)	4.82	0.25	0.25
	assign (segid 3A4 and resid 349 and name CA)	(segid 3A4 and resid 352 and name CG)	5.27	0.42	0.42
	assign (segid 3A4 and resid 349 and name CA)	(segid 3A4 and resid 352 and name N)	4.62	0.11	0.12
	assign (segid 3A4 and resid 349 and name CA)	(segid 3A4 and resid 352 and name O)	6.13	0.14	0.13
	assign (segid 3A4 and resid 349 and name CA)	(segid 3A4 and resid 353 and name CA)	6.34	0.22	0.22
55	assign (segid 3A4 and resid 349 and name CA)	(segid 3A4 and resid 353 and name CB)	6.47	0.28	0.27
	assign (segid 3A4 and resid 349 and name CA)	(segid 3A4 and resid 353 and name CG)	7.43	0.30	0.30
	assign (segid 3A4 and resid 349 and name CA)	(segid 3A4 and resid 353 and name N)	5.56	0.17	0.17
	assign (segid 3A4 and resid 349 and name CA)	(segid 3A4 and resid 354 and name CA)	9.83	0.25	0.25
	assign (segid 3A4 and resid 349 and name CA)	(segid 3A4 and resid 354 and name CB)	10.46	0.32	0.32
60	assign (segid 3A4 and resid 349 and name CA)	(segid 3A4 and resid 355 and name CA)	11.63	0.30	0.29
	assign (segid 3A4 and resid 349 and name CA)	(segid 3A4 and resid 355 and name CB)	11.62	0.41	0.41
	assign (segid 3A4 and resid 349 and name CA)	(segid 3A4 and resid 356 and name CA)	11.09	0.41	0.40
	assign (segid 3A4 and resid 349 and name CA)	(segid 3A4 and resid 356 and name CB)	10.08	0.52	0.53
	assign (segid 3A4 and resid 349 and name CA)	(segid 3A4 and resid 357 and name CA)	11.24	0.12	0.12
65	assign (segid 3A4 and resid 349 and name CA)	(segid 3A4 and resid 357 and name CB)	10.31	0.10	0.10
	assign (segid 3A4 and resid 349 and name CA)	(segid 3A4 and resid 358 and name CA)	13.58	0.10	0.10
	assign (segid 3A4 and resid 349 and name CA)	(segid 3A4 and resid 358 and name CB)	15.00	0.15	0.15
	assign (segid 3A4 and resid 349 and name CA)	(segid 3A4 and resid 359 and name CA)	13.49	0.21	0.21
	assign (segid 3A4 and resid 349 and name CA)	(segid 3A4 and resid 359 and name CB)	14.84	0.19	0.19
70	assign (segid 3A4 and resid 349 and name CA)	(segid 3A4 and resid 360 and name CA)	10.04	0.10	0.11
	assign (segid 3A4 and resid 349 and name CA)	(segid 3A4 and resid 360 and name CB)	8.85	0.16	0.16
	assign (segid 3A4 and resid 349 and name CA)	(segid 3A4 and resid 361 and name CA)	11.01	0.23	0.23
	assign (segid 3A4 and resid 349 and name CA)	(segid 3A4 and resid 361 and name CB)	11.27	0.27	0.26
	assign (segid 3A4 and resid 349 and name CA)	(segid 3A4 and resid 362 and name CA)	14.24	0.20	0.20
75	assign (segid 3A4 and resid 349 and name CA)	(segid 3A4 and resid 362 and name CB)	15.21	0.16	0.16
	assign (segid 3A4 and resid 349 and name CA)	(segid 3A4 and resid 363 and name CA)	15.24	0.34	0.33
	assign (segid 3A4 and resid 349 and name CA)	(segid 3A4 and resid 363 and name CB)	15.78	0.46	0.47
	assign (segid 3A4 and resid 349 and name CA)	(segid 3A4 and resid 364 and name CA)	17.35	0.18	0.19
	assign (segid 3A4 and resid 349 and name CA)	(segid 3A4 and resid 364 and name CB)	17.34	0.16	0.15
80	assign (segid 3A4 and resid 349 and name CA)	(segid 3A4 and resid 365 and name CA)	18.87	0.24	0.24
	assign (segid 3A4 and resid 349 and name CA)	(segid 3A4 and resid 381 and name CA)	10.22	0.76	0.76
	assign (segid 3A4 and resid 349 and name CA)	(segid 3A4 and resid 382 and name CA)	9.64	0.65	0.65
	assign (segid 3A4 and resid 349 and name CA)	(segid 3A4 and resid 382 and name CB)	8.94	0.65	0.64

	assign (segid 3A4 and resid 349 and name CA)	(segid 3A4 and resid 383 and name CA)	10.32	0.68	0.69
	assign (segid 3A4 and resid 349 and name CA)	(segid 3A4 and resid 384 and name CA)	13.52	0.69	0.69
	assign (segid 3A4 and resid 349 and name CA)	(segid 3A4 and resid 384 and name CB)	14.75	0.66	0.67
	assign (segid 3A4 and resid 349 and name CA)	(segid 3A4 and resid 385 and name CA)	12.48	0.80	0.80
	assign (segid 3A4 and resid 349 and name CA)	(segid 3A4 and resid 386 and name CA)	14.21	0.86	0.85
5	assign (segid 3A4 and resid 349 and name CA)	(segid 3A4 and resid 387 and name CA)	17.35	1.07	1.07
	assign (segid 3A4 and resid 349 and name CA)	(segid 3A4 and resid 390 and name CA)	17.21	0.69	0.68
	assign (segid 3A4 and resid 349 and name CA)	(segid 3A4 and resid 390 and name CB)	17.48	0.66	0.66
	assign (segid 3A4 and resid 349 and name CA)	(segid 3A4 and resid 391 and name CA)	18.07	0.69	0.70
	assign (segid 3A4 and resid 349 and name CA)	(segid 3A4 and resid 391 and name CB)	17.34	0.72	0.72
10	assign (segid 3A4 and resid 349 and name CA)	(segid 3A4 and resid 426 and name CA)	17.79	1.19	1.19
	assign (segid 3A4 and resid 349 and name CA)	(segid 3A4 and resid 427 and name CA)	16.99	0.77	0.77
	assign (segid 3A4 and resid 349 and name CA)	(segid 3A4 and resid 428 and name CA)	16.71	0.87	0.88
	assign (segid 3A4 and resid 349 and name CA)	(segid 3A4 and resid 429 and name CA)	15.49	1.28	1.29
	assign (segid 3A4 and resid 349 and name CA)	(segid 3A4 and resid 430 and name CA)	14.62	2.01	2.02
15	assign (segid 3A4 and resid 349 and name CA)	(segid 3A4 and resid 431 and name CA)	14.36	1.18	1.17
	assign (segid 3A4 and resid 349 and name CA)	(segid 3A4 and resid 433 and name CA)	13.54	0.70	0.70
	assign (segid 3A4 and resid 349 and name CA)	(segid 3A4 and resid 434 and name CA)	16.09	0.99	0.99
	assign (segid 3A4 and resid 349 and name CA)	(segid 3A4 and resid 435 and name CA)	18.56	0.63	0.63
	assign (segid 3A4 and resid 349 and name CA)	(segid 3A4 and resid 350 and name C)	5.42	0.09	0.10
20	assign (segid 3A4 and resid 349 and name CB)	(segid 3A4 and resid 350 and name CA)	4.49	0.08	0.07
	assign (segid 3A4 and resid 349 and name CB)	(segid 3A4 and resid 350 and name CB)	5.42	0.16	0.15
	assign (segid 3A4 and resid 349 and name CB)	(segid 3A4 and resid 350 and name N)	3.19	0.12	0.11
	assign (segid 3A4 and resid 349 and name CB)	(segid 3A4 and resid 350 and name O)	6.30	0.09	0.09
	assign (segid 3A4 and resid 349 and name CB)	(segid 3A4 and resid 351 and name C)	6.90	0.16	0.16
25	assign (segid 3A4 and resid 349 and name CB)	(segid 3A4 and resid 351 and name CA)	6.82	0.14	0.14
	assign (segid 3A4 and resid 349 and name CB)	(segid 3A4 and resid 351 and name N)	5.63	0.13	0.13
	assign (segid 3A4 and resid 349 and name CB)	(segid 3A4 and resid 352 and name C)	6.49	0.14	0.14
	assign (segid 3A4 and resid 349 and name CB)	(segid 3A4 and resid 352 and name CA)	6.42	0.24	0.24
	assign (segid 3A4 and resid 349 and name CB)	(segid 3A4 and resid 352 and name CB)	5.99	0.38	0.38
30	assign (segid 3A4 and resid 349 and name CB)	(segid 3A4 and resid 352 and name CG)	6.57	0.52	0.51
	assign (segid 3A4 and resid 349 and name CB)	(segid 3A4 and resid 352 and name N)	5.94	0.17	0.17
	assign (segid 3A4 and resid 349 and name CB)	(segid 3A4 and resid 352 and name O)	6.94	0.11	0.11
	assign (segid 3A4 and resid 349 and name CB)	(segid 3A4 and resid 353 and name CA)	6.94	0.32	0.32
	assign (segid 3A4 and resid 349 and name CB)	(segid 3A4 and resid 353 and name CB)	6.94	0.32	0.32
35	assign (segid 3A4 and resid 349 and name CB)	(segid 3A4 and resid 353 and name N)	6.43	0.21	0.21
	assign (segid 3A4 and resid 349 and name CB)	(segid 3A4 and resid 354 and name CA)	10.41	0.20	0.19
	assign (segid 3A4 and resid 349 and name CB)	(segid 3A4 and resid 354 and name CB)	10.92	0.20	0.20
	assign (segid 3A4 and resid 349 and name CB)	(segid 3A4 and resid 355 and name CA)	12.02	0.37	0.36
	assign (segid 3A4 and resid 349 and name CB)	(segid 3A4 and resid 355 and name CB)	11.84	0.48	0.49
40	assign (segid 3A4 and resid 349 and name CB)	(segid 3A4 and resid 356 and name CA)	11.82	0.44	0.43
	assign (segid 3A4 and resid 349 and name CB)	(segid 3A4 and resid 356 and name CB)	10.82	0.53	0.53
	assign (segid 3A4 and resid 349 and name CB)	(segid 3A4 and resid 357 and name CA)	12.29	0.18	0.17
	assign (segid 3A4 and resid 349 and name CB)	(segid 3A4 and resid 357 and name CB)	11.47	0.15	0.15
	assign (segid 3A4 and resid 349 and name CB)	(segid 3A4 and resid 358 and name CA)	14.51	0.10	0.11
45	assign (segid 3A4 and resid 349 and name CB)	(segid 3A4 and resid 358 and name CB)	15.92	0.18	0.19
	assign (segid 3A4 and resid 349 and name CB)	(segid 3A4 and resid 359 and name CA)	14.52	0.21	0.21
	assign (segid 3A4 and resid 349 and name CB)	(segid 3A4 and resid 359 and name CB)	15.90	0.17	0.18
	assign (segid 3A4 and resid 349 and name CB)	(segid 3A4 and resid 360 and name CA)	11.21	0.13	0.14
	assign (segid 3A4 and resid 349 and name CB)	(segid 3A4 and resid 360 and name CB)	9.94	0.17	0.17
50	assign (segid 3A4 and resid 349 and name CB)	(segid 3A4 and resid 361 and name CA)	12.15	0.24	0.25
	assign (segid 3A4 and resid 349 and name CB)	(segid 3A4 and resid 361 and name CB)	12.28	0.28	0.28
	assign (segid 3A4 and resid 349 and name CB)	(segid 3A4 and resid 362 and name CA)	15.50	0.22	0.22
	assign (segid 3A4 and resid 349 and name CB)	(segid 3A4 and resid 362 and name CB)	16.44	0.19	0.20
	assign (segid 3A4 and resid 349 and name CB)	(segid 3A4 and resid 363 and name CA)	16.64	0.36	0.37
55	assign (segid 3A4 and resid 349 and name CB)	(segid 3A4 and resid 363 and name CB)	17.19	0.50	0.50
	assign (segid 3A4 and resid 349 and name CB)	(segid 3A4 and resid 364 and name CA)	18.78	0.20	0.21
	assign (segid 3A4 and resid 349 and name CB)	(segid 3A4 and resid 364 and name CB)	18.73	0.17	0.17
	assign (segid 3A4 and resid 349 and name CB)	(segid 3A4 and resid 381 and name CA)	11.34	0.67	0.67
	assign (segid 3A4 and resid 349 and name CB)	(segid 3A4 and resid 382 and name CA)	10.50	0.57	0.56
60	assign (segid 3A4 and resid 349 and name CB)	(segid 3A4 and resid 382 and name CB)	9.62	0.58	0.59
	assign (segid 3A4 and resid 349 and name CB)	(segid 3A4 and resid 383 and name CA)	11.34	0.59	0.59
	assign (segid 3A4 and resid 349 and name CB)	(segid 3A4 and resid 384 and name CA)	14.33	0.61	0.61
	assign (segid 3A4 and resid 349 and name CB)	(segid 3A4 and resid 384 and name CB)	15.61	0.58	0.58
	assign (segid 3A4 and resid 349 and name CB)	(segid 3A4 and resid 385 and name CA)	12.95	0.78	0.78
65	assign (segid 3A4 and resid 349 and name CB)	(segid 3A4 and resid 386 and name CA)	14.53	0.82	0.83
	assign (segid 3A4 and resid 349 and name CB)	(segid 3A4 and resid 387 and name CA)	17.49	1.15	1.14
	assign (segid 3A4 and resid 349 and name CB)	(segid 3A4 and resid 390 and name CA)	17.63	0.68	0.68
	assign (segid 3A4 and resid 349 and name CB)	(segid 3A4 and resid 390 and name CB)	17.96	0.68	0.67
	assign (segid 3A4 and resid 349 and name CB)	(segid 3A4 and resid 391 and name CA)	18.67	0.64	0.64
70	assign (segid 3A4 and resid 349 and name CB)	(segid 3A4 and resid 391 and name CB)	18.03	0.65	0.64
	assign (segid 3A4 and resid 349 and name CB)	(segid 3A4 and resid 427 and name CA)	17.47	0.80	0.81
	assign (segid 3A4 and resid 349 and name CB)	(segid 3A4 and resid 428 and name CA)	16.95	0.90	0.91
	assign (segid 3A4 and resid 349 and name CB)	(segid 3A4 and resid 429 and name CA)	15.60	1.42	1.42
	assign (segid 3A4 and resid 349 and name CB)	(segid 3A4 and resid 430 and name CA)	14.55	2.14	2.14
75	assign (segid 3A4 and resid 349 and name CB)	(segid 3A4 and resid 431 and name CA)	14.40	1.22	1.23
	assign (segid 3A4 and resid 349 and name CB)	(segid 3A4 and resid 433 and name CA)	14.14	0.75	0.75
	assign (segid 3A4 and resid 349 and name CB)	(segid 3A4 and resid 434 and name CA)	16.87	1.03	1.03
	assign (segid 3A4 and resid 349 and name CB)	(segid 3A4 and resid 349 and name C)	2.46	0.03	0.02
	assign (segid 3A4 and resid 349 and name N)	(segid 3A4 and resid 349 and name CA)	1.46	0.01	0.00
80	assign (segid 3A4 and resid 349 and name N)	(segid 3A4 and resid 349 and name CB)	2.44	0.02	0.02
	assign (segid 3A4 and resid 349 and name N)	(segid 3A4 and resid 349 and name O)	3.50	0.05	0.05
	assign (segid 3A4 and resid 349 and name N)	(segid 3A4 and resid 350 and name C)	4.78	0.14	0.14

	assign (segid 3A4 and resid 349 and name N) (segid 3A4 and resid 350 and name CA)	4.24	0.09	0.09
	assign (segid 3A4 and resid 349 and name N) (segid 3A4 and resid 350 and name CB)	4.99	0.14	0.13
	assign (segid 3A4 and resid 349 and name N) (segid 3A4 and resid 350 and name N)	2.84	0.08	0.08
	assign (segid 3A4 and resid 349 and name N) (segid 3A4 and resid 350 and name O)	5.88	0.12	0.13
5	assign (segid 3A4 and resid 349 and name N) (segid 3A4 and resid 351 and name C)	5.74	0.19	0.19
	assign (segid 3A4 and resid 349 and name N) (segid 3A4 and resid 351 and name CA)	5.45	0.23	0.23
	assign (segid 3A4 and resid 349 and name N) (segid 3A4 and resid 351 and name N)	4.41	0.19	0.19
	assign (segid 3A4 and resid 349 and name N) (segid 3A4 and resid 351 and name O)	6.87	0.22	0.22
10	assign (segid 3A4 and resid 349 and name N) (segid 3A4 and resid 352 and name C)	6.44	0.20	0.20
	assign (segid 3A4 and resid 349 and name N) (segid 3A4 and resid 352 and name CA)	5.83	0.12	0.13
	assign (segid 3A4 and resid 349 and name N) (segid 3A4 and resid 352 and name CB)	5.38	0.12	0.13
	assign (segid 3A4 and resid 349 and name N) (segid 3A4 and resid 352 and name CG)	5.47	0.21	0.21
	assign (segid 3A4 and resid 349 and name N) (segid 3A4 and resid 352 and name N)	5.05	0.14	0.14
	assign (segid 3A4 and resid 349 and name N) (segid 3A4 and resid 352 and name O)	7.14	0.26	0.26
15	assign (segid 3A4 and resid 349 and name N) (segid 3A4 and resid 353 and name CA)	7.46	0.25	0.25
	assign (segid 3A4 and resid 349 and name N) (segid 3A4 and resid 353 and name N)	6.52	0.20	0.21
	assign (segid 3A4 and resid 349 and name O) (segid 3A4 and resid 349 and name CB)	3.19	0.08	0.08
	assign (segid 3A4 and resid 349 and name O) (segid 3A4 and resid 350 and name C)	2.98	0.14	0.14
	assign (segid 3A4 and resid 349 and name O) (segid 3A4 and resid 350 and name CA)	2.76	0.03	0.04
20	assign (segid 3A4 and resid 349 and name O) (segid 3A4 and resid 350 and name CB)	4.25	0.05	0.04
	assign (segid 3A4 and resid 349 and name O) (segid 3A4 and resid 350 and name N)	2.23	0.02	0.02
	assign (segid 3A4 and resid 349 and name O) (segid 3A4 and resid 350 and name O)	3.52	0.09	0.10
	assign (segid 3A4 and resid 349 and name O) (segid 3A4 and resid 351 and name C)	4.21	0.31	0.32
	assign (segid 3A4 and resid 349 and name O) (segid 3A4 and resid 351 and name CA)	4.41	0.28	0.28
25	assign (segid 3A4 and resid 349 and name O) (segid 3A4 and resid 351 and name N)	3.43	0.24	0.24
	assign (segid 3A4 and resid 349 and name O) (segid 3A4 and resid 351 and name O)	5.32	0.28	0.29
	assign (segid 3A4 and resid 349 and name O) (segid 3A4 and resid 352 and name C)	3.67	0.18	0.18
	assign (segid 3A4 and resid 349 and name O) (segid 3A4 and resid 352 and name CA)	3.76	0.34	0.34
	assign (segid 3A4 and resid 349 and name O) (segid 3A4 and resid 352 and name CB)	3.97	0.46	0.47
30	assign (segid 3A4 and resid 349 and name O) (segid 3A4 and resid 352 and name CG)	4.93	0.57	0.58
	assign (segid 3A4 and resid 349 and name O) (segid 3A4 and resid 352 and name N)	3.20	0.36	0.36
	assign (segid 3A4 and resid 349 and name O) (segid 3A4 and resid 352 and name O)	4.41	0.19	0.19
	assign (segid 3A4 and resid 349 and name O) (segid 3A4 and resid 353 and name C)	5.51	0.13	0.14
	assign (segid 3A4 and resid 349 and name O) (segid 3A4 and resid 353 and name CA)	4.08	0.17	0.16
35	assign (segid 3A4 and resid 349 and name O) (segid 3A4 and resid 353 and name CB)	4.17	0.28	0.28
	assign (segid 3A4 and resid 349 and name O) (segid 3A4 and resid 353 and name CG)	5.25	0.32	0.32
	assign (segid 3A4 and resid 349 and name O) (segid 3A4 and resid 353 and name N)	3.38	0.12	0.12
	assign (segid 3A4 and resid 349 and name O) (segid 3A4 and resid 353 and name O)	6.16	0.16	0.17
40	assign (segid 3A4 and resid 349 and name O) (segid 3A4 and resid 353 and name OD1)	6.15	0.27	0.26
	assign (segid 3A4 and resid 349 and name O) (segid 3A4 and resid 354 and name CA)	7.69	0.15	0.15
	assign (segid 3A4 and resid 349 and name O) (segid 3A4 and resid 354 and name N)	6.28	0.17	0.16
	assign (segid 3A4 and resid 349 and name O) (segid 3A4 and resid 360 and name CB)	7.29	0.29	0.30
	assign (segid 3A4 and resid 34 and name C) (segid 3A4 and resid 344 and name O)	7.73	0.10	0.11
45	assign (segid 3A4 and resid 34 and name C) (segid 3A4 and resid 345 and name C)	7.35	0.30	0.30
	assign (segid 3A4 and resid 34 and name C) (segid 3A4 and resid 345 and name CA)	7.52	0.24	0.25
	assign (segid 3A4 and resid 34 and name C) (segid 3A4 and resid 346 and name C)	6.37	0.52	0.52
	assign (segid 3A4 and resid 34 and name C) (segid 3A4 and resid 346 and name CA)	6.52	0.51	0.51
	assign (segid 3A4 and resid 34 and name C) (segid 3A4 and resid 346 and name CB)	5.91	0.55	0.55
50	assign (segid 3A4 and resid 34 and name C) (segid 3A4 and resid 346 and name N)	6.32	0.39	0.39
	assign (segid 3A4 and resid 34 and name C) (segid 3A4 and resid 346 and name O)	5.44	0.52	0.53
	assign (segid 3A4 and resid 34 and name C) (segid 3A4 and resid 349 and name C)	5.13	0.48	0.47
	assign (segid 3A4 and resid 34 and name C) (segid 3A4 and resid 349 and name CA)	5.47	0.29	0.28
	assign (segid 3A4 and resid 34 and name C) (segid 3A4 and resid 349 and name CB)	4.44	0.22	0.22
55	assign (segid 3A4 and resid 34 and name C) (segid 3A4 and resid 349 and name N)	6.42	0.31	0.30
	assign (segid 3A4 and resid 34 and name C) (segid 3A4 and resid 349 and name O)	5.31	0.39	0.40
	assign (segid 3A4 and resid 34 and name C) (segid 3A4 and resid 34 and name CB)	2.48	0.05	0.06
	assign (segid 3A4 and resid 34 and name C) (segid 3A4 and resid 34 and name O)	1.24	0.01	0.01
	assign (segid 3A4 and resid 34 and name C) (segid 3A4 and resid 350 and name CA)	5.39	0.84	0.84
60	assign (segid 3A4 and resid 34 and name C) (segid 3A4 and resid 350 and name CB)	5.88	0.93	0.92
	assign (segid 3A4 and resid 34 and name C) (segid 3A4 and resid 350 and name N)	5.13	0.71	0.71
	assign (segid 3A4 and resid 34 and name C) (segid 3A4 and resid 35 and name C)	3.23	0.15	0.16
	assign (segid 3A4 and resid 34 and name C) (segid 3A4 and resid 35 and name CA)	2.41	0.02	0.03
	assign (segid 3A4 and resid 34 and name C) (segid 3A4 and resid 35 and name N)	1.32	0.01	0.01
65	assign (segid 3A4 and resid 34 and name C) (segid 3A4 and resid 35 and name O)	3.51	0.29	0.29
	assign (segid 3A4 and resid 34 and name C) (segid 3A4 and resid 36 and name C)	6.14	0.20	0.20
	assign (segid 3A4 and resid 34 and name C) (segid 3A4 and resid 36 and name CA)	5.36	0.15	0.16
	assign (segid 3A4 and resid 34 and name C) (segid 3A4 and resid 36 and name N)	4.22	0.11	0.10
	assign (segid 3A4 and resid 34 and name C) (segid 3A4 and resid 36 and name O)	6.80	0.30	0.30
70	assign (segid 3A4 and resid 34 and name C) (segid 3A4 and resid 37 and name C)	7.32	0.29	0.30
	assign (segid 3A4 and resid 34 and name C) (segid 3A4 and resid 37 and name CA)	7.47	0.23	0.23
	assign (segid 3A4 and resid 34 and name C) (segid 3A4 and resid 37 and name N)	6.41	0.18	0.18
	assign (segid 3A4 and resid 34 and name C) (segid 3A4 and resid 38 and name C)	6.66	0.35	0.34
	assign (segid 3A4 and resid 34 and name C) (segid 3A4 and resid 38 and name CA)	6.50	0.37	0.38
	assign (segid 3A4 and resid 34 and name C) (segid 3A4 and resid 38 and name CB)	5.74	0.16	0.17
75	assign (segid 3A4 and resid 34 and name C) (segid 3A4 and resid 38 and name N)	6.30	0.32	0.32
	assign (segid 3A4 and resid 34 and name C) (segid 3A4 and resid 39 and name CA)	6.50	0.27	0.28
	assign (segid 3A4 and resid 34 and name C) (segid 3A4 and resid 39 and name CB)	5.84	0.26	0.26
	assign (segid 3A4 and resid 34 and name C) (segid 3A4 and resid 39 and name N)	5.94	0.29	0.28
80	assign (segid 3A4 and resid 34 and name CA) (segid 3A4 and resid 313 and name CA)	17.50	0.75	0.76
	assign (segid 3A4 and resid 34 and name CA) (segid 3A4 and resid 313 and name CB)	17.92	0.74	0.73
	assign (segid 3A4 and resid 34 and name CA) (segid 3A4 and resid 314 and name CA)	14.84	0.70	0.71
	assign (segid 3A4 and resid 34 and name CA) (segid 3A4 and resid 314 and name CB)	15.19	0.64	0.64
	assign (segid 3A4 and resid 34 and name CA) (segid 3A4 and resid 315 and name CA)	15.42	0.91	0.91

	assign (segid 3A4 and resid 34 and name CA) (segid 3A4 and resid 315 and name CB)	16.78	0.92	0.92
	assign (segid 3A4 and resid 34 and name CA) (segid 3A4 and resid 316 and name CA)	15.88	1.09	1.10
	assign (segid 3A4 and resid 34 and name CA) (segid 3A4 and resid 317 and name CA)	13.81	0.43	0.42
	assign (segid 3A4 and resid 34 and name CA) (segid 3A4 and resid 318 and name CA)	15.81	0.56	0.57
	assign (segid 3A4 and resid 34 and name CA) (segid 3A4 and resid 318 and name CB)	17.17	0.47	0.48
5	assign (segid 3A4 and resid 34 and name CA) (segid 3A4 and resid 319 and name CA)	14.23	0.47	0.47
	assign (segid 3A4 and resid 34 and name CA) (segid 3A4 and resid 319 and name CB)	14.70	0.59	0.60
	assign (segid 3A4 and resid 34 and name CA) (segid 3A4 and resid 322 and name CA)	12.79	0.44	0.45
	assign (segid 3A4 and resid 34 and name CA) (segid 3A4 and resid 323 and name CA)	13.97	0.24	0.25
	assign (segid 3A4 and resid 34 and name CA) (segid 3A4 and resid 323 and name CB)	13.26	0.44	0.44
10	assign (segid 3A4 and resid 34 and name CA) (segid 3A4 and resid 324 and name CA)	16.20	0.30	0.29
	assign (segid 3A4 and resid 34 and name CA) (segid 3A4 and resid 324 and name CB)	17.55	0.33	0.33
	assign (segid 3A4 and resid 34 and name CA) (segid 3A4 and resid 325 and name CA)	16.86	0.24	0.25
	assign (segid 3A4 and resid 34 and name CA) (segid 3A4 and resid 325 and name CB)	16.45	0.29	0.29
	assign (segid 3A4 and resid 34 and name CA) (segid 3A4 and resid 329 and name CA)	17.35	0.70	0.70
15	assign (segid 3A4 and resid 34 and name CA) (segid 3A4 and resid 329 and name CB)	16.60	0.74	0.74
	assign (segid 3A4 and resid 34 and name CA) (segid 3A4 and resid 330 and name CA)	15.84	0.74	0.74
	assign (segid 3A4 and resid 34 and name CA) (segid 3A4 and resid 330 and name CB)	16.91	0.77	0.78
	assign (segid 3A4 and resid 34 and name CA) (segid 3A4 and resid 331 and name CA)	12.35	0.77	0.77
	assign (segid 3A4 and resid 34 and name CA) (segid 3A4 and resid 331 and name CB)	11.32	0.77	0.77
20	assign (segid 3A4 and resid 34 and name CA) (segid 3A4 and resid 332 and name CA)	11.93	0.89	0.89
	assign (segid 3A4 and resid 34 and name CA) (segid 3A4 and resid 333 and name CA)	14.71	0.88	0.88
	assign (segid 3A4 and resid 34 and name CA) (segid 3A4 and resid 335 and name CA)	13.67	0.62	0.61
	assign (segid 3A4 and resid 34 and name CA) (segid 3A4 and resid 336 and name CA)	16.06	0.51	0.51
	assign (segid 3A4 and resid 34 and name CA) (segid 3A4 and resid 336 and name CB)	17.45	0.48	0.48
25	assign (segid 3A4 and resid 34 and name CA) (segid 3A4 and resid 337 and name CA)	15.30	0.62	0.62
	assign (segid 3A4 and resid 34 and name CA) (segid 3A4 and resid 337 and name CB)	14.29	0.60	0.60
	assign (segid 3A4 and resid 34 and name CA) (segid 3A4 and resid 338 and name CA)	18.61	0.52	0.51
	assign (segid 3A4 and resid 34 and name CA) (segid 3A4 and resid 341 and name CA)	16.46	0.23	0.24
	assign (segid 3A4 and resid 34 and name CA) (segid 3A4 and resid 341 and name CB)	15.74	0.34	0.33
30	assign (segid 3A4 and resid 34 and name CA) (segid 3A4 and resid 342 and name CA)	14.34	0.14	0.15
	assign (segid 3A4 and resid 34 and name CA) (segid 3A4 and resid 343 and name CA)	10.73	0.17	0.18
	assign (segid 3A4 and resid 34 and name CA) (segid 3A4 and resid 343 and name CB)	10.54	0.22	0.23
	assign (segid 3A4 and resid 34 and name CA) (segid 3A4 and resid 344 and name C)	7.60	0.14	0.14
	assign (segid 3A4 and resid 34 and name CA) (segid 3A4 and resid 344 and name CA)	8.88	0.14	0.13
35	assign (segid 3A4 and resid 34 and name CA) (segid 3A4 and resid 344 and name CB)	9.03	0.27	0.28
	assign (segid 3A4 and resid 34 and name CA) (segid 3A4 and resid 344 and name O)	6.60	0.13	0.14
	assign (segid 3A4 and resid 34 and name CA) (segid 3A4 and resid 345 and name C)	6.66	0.42	0.41
	assign (segid 3A4 and resid 34 and name CA) (segid 3A4 and resid 345 and name CA)	6.80	0.34	0.33
	assign (segid 3A4 and resid 34 and name CA) (segid 3A4 and resid 345 and name CB)	7.63	0.48	0.48
40	assign (segid 3A4 and resid 34 and name CA) (segid 3A4 and resid 346 and name C)	6.04	0.66	0.65
	assign (segid 3A4 and resid 34 and name CA) (segid 3A4 and resid 346 and name CA)	5.84	0.63	0.64
	assign (segid 3A4 and resid 34 and name CA) (segid 3A4 and resid 346 and name CB)	5.08	0.65	0.64
	assign (segid 3A4 and resid 34 and name CA) (segid 3A4 and resid 346 and name N)	5.57	0.50	0.50
	assign (segid 3A4 and resid 34 and name CA) (segid 3A4 and resid 346 and name O)	5.31	0.64	0.65
45	assign (segid 3A4 and resid 34 and name CA) (segid 3A4 and resid 347 and name CA)	7.98	0.68	0.68
	assign (segid 3A4 and resid 34 and name CA) (segid 3A4 and resid 347 and name CB)	9.44	0.68	0.69
	assign (segid 3A4 and resid 34 and name CA) (segid 3A4 and resid 348 and name CA)	8.67	0.48	0.48
	assign (segid 3A4 and resid 34 and name CA) (segid 3A4 and resid 349 and name C)	5.71	0.65	0.64
	assign (segid 3A4 and resid 34 and name CA) (segid 3A4 and resid 349 and name CA)	5.67	0.47	0.47
50	assign (segid 3A4 and resid 34 and name CA) (segid 3A4 and resid 349 and name CB)	4.39	0.38	0.38
	assign (segid 3A4 and resid 34 and name CA) (segid 3A4 and resid 349 and name N)	6.47	0.47	0.47
	assign (segid 3A4 and resid 34 and name CA) (segid 3A4 and resid 349 and name O)	6.10	0.54	0.53
	assign (segid 3A4 and resid 34 and name CA) (segid 3A4 and resid 34 and name C)	1.52	0.02	0.01
	assign (segid 3A4 and resid 34 and name CA) (segid 3A4 and resid 34 and name CB)	1.53	0.03	0.04
55	assign (segid 3A4 and resid 34 and name CA) (segid 3A4 and resid 34 and name O)	2.39	0.02	0.01
	assign (segid 3A4 and resid 34 and name CA) (segid 3A4 and resid 350 and name CA)	6.31	0.93	0.94
	assign (segid 3A4 and resid 34 and name CA) (segid 3A4 and resid 350 and name CB)	6.72	1.04	1.04
	assign (segid 3A4 and resid 34 and name CA) (segid 3A4 and resid 350 and name N)	5.76	0.88	0.87
	assign (segid 3A4 and resid 34 and name CA) (segid 3A4 and resid 351 and name CA)	9.78	0.79	0.79
60	assign (segid 3A4 and resid 34 and name CA) (segid 3A4 and resid 352 and name CA)	9.65	0.74	0.73
	assign (segid 3A4 and resid 34 and name CA) (segid 3A4 and resid 352 and name CB)	9.58	0.75	0.75
	assign (segid 3A4 and resid 34 and name CA) (segid 3A4 and resid 353 and name CA)	8.48	0.77	0.77
	assign (segid 3A4 and resid 34 and name CA) (segid 3A4 and resid 353 and name CB)	7.91	0.85	0.85
	assign (segid 3A4 and resid 34 and name CA) (segid 3A4 and resid 354 and name CA)	11.74	0.70	0.70
65	assign (segid 3A4 and resid 34 and name CA) (segid 3A4 and resid 354 and name CB)	12.13	0.64	0.65
	assign (segid 3A4 and resid 34 and name CA) (segid 3A4 and resid 355 and name CA)	12.28	0.97	0.97
	assign (segid 3A4 and resid 34 and name CA) (segid 3A4 and resid 355 and name CB)	11.61	1.08	1.08
	assign (segid 3A4 and resid 34 and name CA) (segid 3A4 and resid 356 and name CA)	12.72	0.79	0.80
	assign (segid 3A4 and resid 34 and name CA) (segid 3A4 and resid 356 and name CB)	11.74	0.75	0.75
70	assign (segid 3A4 and resid 34 and name CA) (segid 3A4 and resid 357 and name CA)	14.27	0.81	0.80
	assign (segid 3A4 and resid 34 and name CA) (segid 3A4 and resid 357 and name CB)	13.81	0.86	0.86
	assign (segid 3A4 and resid 34 and name CA) (segid 3A4 and resid 358 and name CA)	16.57	0.62	0.62
	assign (segid 3A4 and resid 34 and name CA) (segid 3A4 and resid 358 and name CB)	17.89	0.69	0.70
	assign (segid 3A4 and resid 34 and name CA) (segid 3A4 and resid 359 and name CA)	17.17	0.63	0.63
75	assign (segid 3A4 and resid 34 and name CA) (segid 3A4 and resid 35 and name C)	4.58	0.11	0.11
	assign (segid 3A4 and resid 34 and name CA) (segid 3A4 and resid 35 and name CA)	3.81	0.02	0.01
	assign (segid 3A4 and resid 34 and name CA) (segid 3A4 and resid 35 and name N)	2.46	0.01	0.00
	assign (segid 3A4 and resid 34 and name CA) (segid 3A4 and resid 35 and name O)	4.59	0.26	0.25
	assign (segid 3A4 and resid 34 and name CA) (segid 3A4 and resid 360 and name CA)	14.28	0.62	0.62
80	assign (segid 3A4 and resid 34 and name CA) (segid 3A4 and resid 360 and name CB)	12.86	0.61	0.61
	assign (segid 3A4 and resid 34 and name CA) (segid 3A4 and resid 361 and name CA)	15.73	0.65	0.64
	assign (segid 3A4 and resid 34 and name CA) (segid 3A4 and resid 361 and name CB)	15.78	0.65	0.65

	assign	(segid 3A4 and resid 34 and name CA)	(segid 3A4 and resid 36 and name C)	7.38	0.19	0.20
	assign	(segid 3A4 and resid 34 and name CA)	(segid 3A4 and resid 36 and name CA)	6.71	0.13	0.13
	assign	(segid 3A4 and resid 34 and name CA)	(segid 3A4 and resid 36 and name N)	5.65	0.08	0.08
	assign	(segid 3A4 and resid 34 and name CA)	(segid 3A4 and resid 37 and name CA)	8.64	0.24	0.24
5	assign	(segid 3A4 and resid 34 and name CA)	(segid 3A4 and resid 37 and name CB)	9.13	0.34	0.33
	assign	(segid 3A4 and resid 34 and name CA)	(segid 3A4 and resid 37 and name N)	7.69	0.17	0.18
	assign	(segid 3A4 and resid 34 and name CA)	(segid 3A4 and resid 381 and name CA)	13.35	0.69	0.69
	assign	(segid 3A4 and resid 34 and name CA)	(segid 3A4 and resid 382 and name CA)	12.15	0.50	0.51
	assign	(segid 3A4 and resid 34 and name CA)	(segid 3A4 and resid 382 and name CB)	10.90	0.55	0.54
10	assign	(segid 3A4 and resid 34 and name CA)	(segid 3A4 and resid 383 and name CA)	13.86	0.37	0.37
	assign	(segid 3A4 and resid 34 and name CA)	(segid 3A4 and resid 384 and name CA)	16.20	0.37	0.37
	assign	(segid 3A4 and resid 34 and name CA)	(segid 3A4 and resid 384 and name CB)	17.48	0.37	0.37
	assign	(segid 3A4 and resid 34 and name CA)	(segid 3A4 and resid 385 and name CA)	13.92	0.52	0.52
	assign	(segid 3A4 and resid 34 and name CA)	(segid 3A4 and resid 386 and name CA)	14.61	0.40	0.39
15	assign	(segid 3A4 and resid 34 and name CA)	(segid 3A4 and resid 387 and name CA)	16.88	0.92	0.92
	assign	(segid 3A4 and resid 34 and name CA)	(segid 3A4 and resid 389 and name CA)	18.85	0.58	0.58
	assign	(segid 3A4 and resid 34 and name CA)	(segid 3A4 and resid 389 and name CB)	18.08	0.59	0.60
	assign	(segid 3A4 and resid 34 and name CA)	(segid 3A4 and resid 38 and name C)	7.13	0.37	0.38
	assign	(segid 3A4 and resid 34 and name CA)	(segid 3A4 and resid 38 and name CA)	7.10	0.40	0.40
20	assign	(segid 3A4 and resid 34 and name CA)	(segid 3A4 and resid 38 and name CB)	6.15	0.48	0.49
	assign	(segid 3A4 and resid 34 and name CA)	(segid 3A4 and resid 38 and name N)	7.18	0.33	0.33
	assign	(segid 3A4 and resid 34 and name CA)	(segid 3A4 and resid 390 and name CA)	18.20	0.60	0.61
	assign	(segid 3A4 and resid 34 and name CA)	(segid 3A4 and resid 390 and name CB)	18.50	0.67	0.68
	assign	(segid 3A4 and resid 34 and name CA)	(segid 3A4 and resid 39 and name CA)	6.92	0.30	0.30
25	assign	(segid 3A4 and resid 34 and name CA)	(segid 3A4 and resid 39 and name CB)	6.32	0.28	0.28
	assign	(segid 3A4 and resid 34 and name CA)	(segid 3A4 and resid 39 and name N)	6.50	0.30	0.30
	assign	(segid 3A4 and resid 34 and name CA)	(segid 3A4 and resid 40 and name CA)	10.41	0.27	0.27
	assign	(segid 3A4 and resid 34 and name CA)	(segid 3A4 and resid 40 and name CB)	10.99	0.25	0.26
	assign	(segid 3A4 and resid 34 and name CA)	(segid 3A4 and resid 41 and name CA)	11.55	0.30	0.30
30	assign	(segid 3A4 and resid 34 and name CA)	(segid 3A4 and resid 41 and name CB)	11.21	0.34	0.35
	assign	(segid 3A4 and resid 34 and name CA)	(segid 3A4 and resid 42 and name CA)	10.94	0.32	0.33
	assign	(segid 3A4 and resid 34 and name CA)	(segid 3A4 and resid 42 and name CB)	9.74	0.32	0.33
	assign	(segid 3A4 and resid 34 and name CA)	(segid 3A4 and resid 431 and name CA)	16.53	1.22	1.22
	assign	(segid 3A4 and resid 34 and name CA)	(segid 3A4 and resid 433 and name CA)	17.55	0.56	0.56
35	assign	(segid 3A4 and resid 34 and name CB)	(segid 3A4 and resid 313 and name CA)	18.21	0.87	0.87
	assign	(segid 3A4 and resid 34 and name CB)	(segid 3A4 and resid 313 and name CB)	18.73	0.85	0.84
	assign	(segid 3A4 and resid 34 and name CB)	(segid 3A4 and resid 314 and name CA)	15.48	0.80	0.81
	assign	(segid 3A4 and resid 34 and name CB)	(segid 3A4 and resid 314 and name CB)	15.81	0.75	0.75
	assign	(segid 3A4 and resid 34 and name CB)	(segid 3A4 and resid 315 and name CA)	15.71	1.02	1.02
40	assign	(segid 3A4 and resid 34 and name CB)	(segid 3A4 and resid 315 and name CB)	17.01	1.04	1.04
	assign	(segid 3A4 and resid 34 and name CB)	(segid 3A4 and resid 316 and name CA)	16.20	1.21	1.20
	assign	(segid 3A4 and resid 34 and name CB)	(segid 3A4 and resid 317 and name CA)	14.38	0.48	0.48
	assign	(segid 3A4 and resid 34 and name CB)	(segid 3A4 and resid 318 and name CA)	16.38	0.47	0.47
	assign	(segid 3A4 and resid 34 and name CB)	(segid 3A4 and resid 318 and name CB)	17.77	0.39	0.39
45	assign	(segid 3A4 and resid 34 and name CB)	(segid 3A4 and resid 319 and name CA)	14.98	0.41	0.41
	assign	(segid 3A4 and resid 34 and name CB)	(segid 3A4 and resid 319 and name CB)	15.57	0.55	0.55
	assign	(segid 3A4 and resid 34 and name CB)	(segid 3A4 and resid 322 and name CA)	13.77	0.34	0.33
	assign	(segid 3A4 and resid 34 and name CB)	(segid 3A4 and resid 323 and name CA)	15.05	0.28	0.27
	assign	(segid				

	assign (segid 3A4 and resid 34 and name CB) (segid 3A4 and resid 349 and name CB)	4.54	0.68	0.68
	assign (segid 3A4 and resid 34 and name CB) (segid 3A4 and resid 349 and name O)	6.40	0.74	0.74
	assign (segid 3A4 and resid 34 and name CB) (segid 3A4 and resid 350 and name CA)	7.20	1.04	1.04
	assign (segid 3A4 and resid 34 and name CB) (segid 3A4 and resid 350 and name CB)	7.84	1.11	1.11
	assign (segid 3A4 and resid 34 and name CB) (segid 3A4 and resid 351 and name CA)	10.42	0.91	0.91
5	assign (segid 3A4 and resid 34 and name CB) (segid 3A4 and resid 352 and name CA)	9.74	0.87	0.87
	assign (segid 3A4 and resid 34 and name CB) (segid 3A4 and resid 352 and name CB)	9.52	0.90	0.89
	assign (segid 3A4 and resid 34 and name CB) (segid 3A4 and resid 353 and name CA)	8.60	0.85	0.85
	assign (segid 3A4 and resid 34 and name CB) (segid 3A4 and resid 353 and name CB)	8.26	0.90	0.90
	assign (segid 3A4 and resid 34 and name CB) (segid 3A4 and resid 354 and name CA)	11.60	0.77	0.76
10	assign (segid 3A4 and resid 34 and name CB) (segid 3A4 and resid 354 and name CB)	11.81	0.71	0.71
	assign (segid 3A4 and resid 34 and name CB) (segid 3A4 and resid 355 and name CA)	12.42	1.00	0.99
	assign (segid 3A4 and resid 34 and name CB) (segid 3A4 and resid 355 and name CB)	11.78	1.10	1.09
	assign (segid 3A4 and resid 34 and name CB) (segid 3A4 and resid 356 and name CA)	13.22	0.82	0.82
	assign (segid 3A4 and resid 34 and name CB) (segid 3A4 and resid 356 and name CB)	12.37	0.76	0.76
15	assign (segid 3A4 and resid 34 and name CB) (segid 3A4 and resid 357 and name CA)	14.57	0.86	0.86
	assign (segid 3A4 and resid 34 and name CB) (segid 3A4 and resid 357 and name CB)	14.14	0.94	0.94
	assign (segid 3A4 and resid 34 and name CB) (segid 3A4 and resid 358 and name CA)	16.52	0.72	0.71
	assign (segid 3A4 and resid 34 and name CB) (segid 3A4 and resid 358 and name CB)	17.84	0.82	0.82
	assign (segid 3A4 and resid 34 and name CB) (segid 3A4 and resid 359 and name CA)	16.94	0.67	0.67
20	assign (segid 3A4 and resid 34 and name CB) (segid 3A4 and resid 35 and name C)	5.66	0.15	0.15
	assign (segid 3A4 and resid 34 and name CB) (segid 3A4 and resid 35 and name N)	4.59	0.09	0.10
	assign (segid 3A4 and resid 34 and name CB) (segid 3A4 and resid 35 and name O)	3.37	0.11	0.10
	assign (segid 3A4 and resid 34 and name CB) (segid 3A4 and resid 35 and name N)	5.87	0.27	0.27
	assign (segid 3A4 and resid 34 and name CB) (segid 3A4 and resid 360 and name CA)	14.19	0.69	0.70
25	assign (segid 3A4 and resid 34 and name CB) (segid 3A4 and resid 360 and name CB)	12.75	0.68	0.68
	assign (segid 3A4 and resid 34 and name CB) (segid 3A4 and resid 361 and name CA)	15.42	0.73	0.74
	assign (segid 3A4 and resid 34 and name CB) (segid 3A4 and resid 361 and name CB)	15.34	0.74	0.74
	assign (segid 3A4 and resid 34 and name CB) (segid 3A4 and resid 36 and name CA)	7.83	0.15	0.16
30	assign (segid 3A4 and resid 34 and name CB) (segid 3A4 and resid 36 and name N)	6.65	0.11	0.10
	assign (segid 3A4 and resid 34 and name CB) (segid 3A4 and resid 37 and name CA)	9.73	0.28	0.28
	assign (segid 3A4 and resid 34 and name CB) (segid 3A4 and resid 37 and name CB)	10.04	0.42	0.41
	assign (segid 3A4 and resid 34 and name CB) (segid 3A4 and resid 381 and name CA)	14.41	0.72	0.73
	assign (segid 3A4 and resid 34 and name CB) (segid 3A4 and resid 382 and name CA)	13.40	0.55	0.56
35	assign (segid 3A4 and resid 34 and name CB) (segid 3A4 and resid 382 and name CB)	12.21	0.60	0.59
	assign (segid 3A4 and resid 34 and name CB) (segid 3A4 and resid 383 and name CA)	14.93	0.43	0.44
	assign (segid 3A4 and resid 34 and name CB) (segid 3A4 and resid 384 and name CA)	17.44	0.42	0.42
	assign (segid 3A4 and resid 34 and name CB) (segid 3A4 and resid 384 and name CB)	18.72	0.42	0.43
	assign (segid 3A4 and resid 34 and name CB) (segid 3A4 and resid 385 and name CA)	15.29	0.54	0.55
40	assign (segid 3A4 and resid 34 and name CB) (segid 3A4 and resid 386 and name CA)	16.10	0.40	0.39
	assign (segid 3A4 and resid 34 and name CB) (segid 3A4 and resid 387 and name CA)	18.40	0.93	0.92
	assign (segid 3A4 and resid 34 and name CB) (segid 3A4 and resid 38 and name CA)	8.29	0.42	0.41
	assign (segid 3A4 and resid 34 and name CB) (segid 3A4 and resid 38 and name CB)	7.21	0.51	0.51
	assign (segid 3A4 and resid 34 and name CB) (segid 3A4 and resid 39 and name CA)	8.43	0.30	0.30
	assign (segid 3A4 and resid 34 and name CB) (segid 3A4 and resid 39 and name CB)	7.84	0.30	0.31
45	assign (segid 3A4 and resid 34 and name CB) (segid 3A4 and resid 40 and name CA)	11.88	0.28	0.27
	assign (segid 3A4 and resid 34 and name CB) (segid 3A4 and resid 40 and name CB)	12.41	0.25	0.25
	assign (segid 3A4 and resid 34 and name CB) (segid 3A4 and resid 41 and name CA)	17.91	0.30	0.31
	assign (segid 3A4 and resid 34 and name CB) (segid 3A4 and resid 41 and name CB)	12.49	0.35	0.35
	assign (segid 3A4 and resid 34 and name CB) (segid 3A4 and resid 42 and name CA)	12.32	0.33	0.33
50	assign (segid 3A4 and resid 34 and name CB) (segid 3A4 and resid 42 and name CB)	11.10	0.33	0.33
	assign (segid 3A4 and resid 34 and name CB) (segid 3A4 and resid 431 and name CA)	16.90	1.11	1.12
	assign (segid 3A4 and resid 34 and name CB) (segid 3A4 and resid 433 and name CA)	17.76	0.57	0.58
	assign (segid 3A4 and resid 34 and name N) (segid 3A4 and resid 344 and name C)	6.81	0.14	0.14
55	assign (segid 3A4 and resid 34 and name N) (segid 3A4 and resid 344 and name O)	5.74	0.13	0.14
	assign (segid 3A4 and resid 34 and name N) (segid 3A4 and resid 345 and name C)	6.41	0.36	0.35
	assign (segid 3A4 and resid 34 and name N) (segid 3A4 and resid 345 and name CA)	6.24	0.29	0.29
	assign (segid 3A4 and resid 34 and name N) (segid 3A4 and resid 345 and name CB)	7.06	0.40	0.41
	assign (segid 3A4 and resid 34 and name N) (segid 3A4 and resid 345 and name N)	7.06	0.18	0.18
60	assign (segid 3A4 and resid 34 and name N) (segid 3A4 and resid 346 and name CA)	6.10	0.58	0.57
	assign (segid 3A4 and resid 34 and name N) (segid 3A4 and resid 346 and name CB)	5.48	0.59	0.59
	assign (segid 3A4 and resid 34 and name N) (segid 3A4 and resid 346 and name N)	5.49	0.46	0.46
	assign (segid 3A4 and resid 34 and name N) (segid 3A4 and resid 346 and name O)	5.96	0.54	0.54
	assign (segid 3A4 and resid 34 and name N) (segid 3A4 and resid 349 and name C)	6.97	0.56	0.56
65	assign (segid 3A4 and resid 34 and name N) (segid 3A4 and resid 349 and name CA)	6.93	0.40	0.40
	assign (segid 3A4 and resid 34 and name N) (segid 3A4 and resid 349 and name CB)	5.64	0.33	0.32
	assign (segid 3A4 and resid 34 and name N) (segid 3A4 and resid 34 and name C)	2.52	0.04	0.05
	assign (segid 3A4 and resid 34 and name N) (segid 3A4 and resid 34 and name CA)	1.46	0.01	0.01
	assign (segid 3A4 and resid 34 and name N) (segid 3A4 and resid 34 and name CB)	2.45	0.03	0.02
	assign (segid 3A4 and resid 34 and name N) (segid 3A4 and resid 34 and name O)	3.62	0.03	0.04
70	assign (segid 3A4 and resid 34 and name N) (segid 3A4 and resid 35 and name C)	4.95	0.02	0.03
	assign (segid 3A4 and resid 34 and name N) (segid 3A4 and resid 35 and name CA)	4.30	0.07	0.07
	assign (segid 3A4 and resid 34 and name N) (segid 3A4 and resid 35 and name N)	2.87	0.09	0.09
	assign (segid 3A4 and resid 34 and name N) (segid 3A4 and resid 35 and name O)	4.66	0.14	0.14
75	assign (segid 3A4 and resid 34 and name N) (segid 3A4 and resid 36 and name C)	7.55	0.15	0.15
	assign (segid 3A4 and resid 34 and name N) (segid 3A4 and resid 36 and name CA)	7.14	0.06	0.07
	assign (segid 3A4 and resid 34 and name N) (segid 3A4 and resid 36 and name N)	6.18	0.04	0.04
	assign (segid 3A4 and resid 34 and name N) (segid 3A4 and resid 38 and name C)	6.40	0.35	0.36
	assign (segid 3A4 and resid 34 and name N) (segid 3A4 and resid 38 and name CA)	6.40	0.38	0.39
80	assign (segid 3A4 and resid 34 and name N) (segid 3A4 and resid 38 and name CB)	5.33	0.46	0.45
	assign (segid 3A4 and resid 34 and name N) (segid 3A4 and resid 38 and name N)	6.75	0.30	0.31
	assign (segid 3A4 and resid 34 and name N) (segid 3A4 and resid 38 and name O)	7.10	0.39	0.39
	assign (segid 3A4 and resid 34 and name N) (segid 3A4 and resid 39 and name CA)	6.43	0.26	0.26

	assign (segid 3A4 and resid 34 and name N)	(segid 3A4 and resid 39 and name CB)	6.11	0.25	0.25
	assign (segid 3A4 and resid 34 and name N)	(segid 3A4 and resid 39 and name N)	5.98	0.27	0.27
	assign (segid 3A4 and resid 34 and name O)	(segid 3A4 and resid 346 and name C)	6.15	0.67	0.68
	assign (segid 3A4 and resid 34 and name O)	(segid 3A4 and resid 346 and name CA)	6.52	0.64	0.65
5	assign (segid 3A4 and resid 34 and name O)	(segid 3A4 and resid 346 and name CB)	5.92	0.66	0.66
	assign (segid 3A4 and resid 34 and name O)	(segid 3A4 and resid 346 and name N)	6.56	0.52	0.52
	assign (segid 3A4 and resid 34 and name O)	(segid 3A4 and resid 346 and name O)	5.10	0.68	0.68
	assign (segid 3A4 and resid 34 and name O)	(segid 3A4 and resid 348 and name C)	6.73	0.42	0.43
	assign (segid 3A4 and resid 34 and name O)	(segid 3A4 and resid 349 and name C)	4.09	0.53	0.54
10	assign (segid 3A4 and resid 34 and name O)	(segid 3A4 and resid 349 and name CA)	4.57	0.34	0.34
	assign (segid 3A4 and resid 34 and name O)	(segid 3A4 and resid 349 and name CB)	3.75	0.31	0.31
	assign (segid 3A4 and resid 34 and name O)	(segid 3A4 and resid 349 and name N)	5.62	0.38	0.39
	assign (segid 3A4 and resid 34 and name O)	(segid 3A4 and resid 349 and name O)	4.17	0.44	0.45
	assign (segid 3A4 and resid 34 and name O)	(segid 3A4 and resid 34 and name CB)	3.06	0.11	0.10
15	assign (segid 3A4 and resid 34 and name O)	(segid 3A4 and resid 350 and name C)	5.65	0.84	0.84
	assign (segid 3A4 and resid 34 and name O)	(segid 3A4 and resid 350 and name CA)	4.46	0.89	0.90
	assign (segid 3A4 and resid 34 and name O)	(segid 3A4 and resid 350 and name CB)	5.19	0.96	0.96
	assign (segid 3A4 and resid 34 and name O)	(segid 3A4 and resid 350 and name N)	4.20	0.77	0.77
	assign (segid 3A4 and resid 34 and name O)	(segid 3A4 and resid 350 and name O)	6.04	0.87	0.88
20	assign (segid 3A4 and resid 34 and name O)	(segid 3A4 and resid 351 and name N)	6.57	0.78	0.77
	assign (segid 3A4 and resid 34 and name O)	(segid 3A4 and resid 353 and name CB)	5.57	0.86	0.85
	assign (segid 3A4 and resid 34 and name O)	(segid 3A4 and resid 35 and name C)	3.34	0.28	0.28
	assign (segid 3A4 and resid 34 and name O)	(segid 3A4 and resid 35 and name CA)	2.70	0.06	0.06
	assign (segid 3A4 and resid 34 and name O)	(segid 3A4 and resid 35 and name N)	2.22	0.02	0.02
25	assign (segid 3A4 and resid 34 and name O)	(segid 3A4 and resid 35 and name O)	3.84	0.48	0.47
	assign (segid 3A4 and resid 34 and name O)	(segid 3A4 and resid 36 and name C)	6.12	0.33	0.34
	assign (segid 3A4 and resid 34 and name O)	(segid 3A4 and resid 36 and name CA)	5.10	0.31	0.31
	assign (segid 3A4 and resid 34 and name O)	(segid 3A4 and resid 36 and name N)	3.99	0.21	0.22
	assign (segid 3A4 and resid 34 and name O)	(segid 3A4 and resid 36 and name O)	6.84	0.45	0.46
30	assign (segid 3A4 and resid 34 and name O)	(segid 3A4 and resid 37 and name N)	6.50	0.25	0.26
	assign (segid 3A4 and resid 34 and name O)	(segid 3A4 and resid 38 and name CA)	7.27	0.44	0.44
	assign (segid 3A4 and resid 34 and name O)	(segid 3A4 and resid 38 and name CB)	6.68	0.51	0.51
	assign (segid 3A4 and resid 34 and name O)	(segid 3A4 and resid 38 and name N)	6.89	0.40	0.39
	assign (segid 3A4 and resid 34 and name O)	(segid 3A4 and resid 39 and name CA)	6.97	0.44	0.43
35	assign (segid 3A4 and resid 34 and name O)	(segid 3A4 and resid 39 and name CB)	6.09	0.42	0.41
	assign (segid 3A4 and resid 34 and name O)	(segid 3A4 and resid 39 and name N)	6.50	0.43	0.44
	assign (segid 3A4 and resid 34 and name O)	(segid 3A4 and resid 350 and name CB)	2.48	0.01	0.01
	assign (segid 3A4 and resid 350 and name C)	(segid 3A4 and resid 350 and name O)	1.23	0.02	0.01
	assign (segid 3A4 and resid 350 and name C)	(segid 3A4 and resid 351 and name C)	3.14	0.05	0.04
40	assign (segid 3A4 and resid 350 and name C)	(segid 3A4 and resid 351 and name CA)	2.44	0.01	0.01
	assign (segid 3A4 and resid 350 and name C)	(segid 3A4 and resid 351 and name N)	1.33	0.01	0.01
	assign (segid 3A4 and resid 350 and name C)	(segid 3A4 and resid 351 and name O)	4.24	0.08	0.08
	assign (segid 3A4 and resid 350 and name C)	(segid 3A4 and resid 352 and name C)	4.59	0.08	0.08
	assign (segid 3A4 and resid 350 and name C)	(segid 3A4 and resid 352 and name CA)	4.39	0.07	0.07
45	assign (segid 3A4 and resid 350 and name C)	(segid 3A4 and resid 352 and name CB)	5.29	0.09	0.10
	assign (segid 3A4 and resid 350 and name C)	(segid 3A4 and resid 352 and name CG)	5.91	0.15	0.16
	assign (segid 3A4 and resid 350 and name C)	(segid 3A4 and resid 352 and name N)	3.12	0.07	0.07
	assign (segid 3A4 and resid 350 and name C)	(segid 3A4 and resid 352 and name O)	5.75	0.10	0.10
	assign (segid 3A4 and resid 350 and name C)	(segid 3A4 and resid 353 and name C)	5.82	0.16	0.16
50	assign (segid 3A4 and resid 350 and name C)	(segid 3A4 and resid 353 and name CA)	4.69	0.10	0.10
	assign (segid 3A4 and resid 350 and name C)	(segid 3A4 and resid 353 and name CB)	4.25	0.16	0.16
	assign (segid 3A4 and resid 350 and name C)	(segid 3A4 and resid 353 and name CG)	5.54	0.16	0.16
	assign (segid 3A4 and resid 350 and name C)	(segid 3A4 and resid 353 and name N)	3.85	0.08	0.07
	assign (segid 3A4 and resid 350 and name C)	(segid 3A4 and resid 353 and name O)	5.88	0.26	0.26
55	assign (segid 3A4 and resid 350 and name C)	(segid 3A4 and resid 353 and name OD1)	6.62	0.15	0.16
	assign (segid 3A4 and resid 350 and name C)	(segid 3A4 and resid 354 and name N)	7.00	0.13	0.13
	assign (segid 3A4 and resid 350 and name C)	(segid 3A4 and resid 356 and name CB)	6.27	0.62	0.61
	assign (segid 3A4 and resid 350 and name C)	(segid 3A4 and resid 357 and name CB)	7.20	0.22	0.22
	assign (segid 3A4 and resid 350 and name C)	(segid 3A4 and resid 357 and name N)	7.44	0.38	0.38
60	assign (segid 3A4 and resid 350 and name C)	(segid 3A4 and resid 381 and name C)	6.81	0.53	0.53
	assign (segid 3A4 and resid 350 and name C)	(segid 3A4 and resid 381 and name CA)	6.43	0.55	0.55
	assign (segid 3A4 and resid 350 and name C)	(segid 3A4 and resid 381 and name N)	6.96	0.69	0.69
	assign (segid 3A4 and resid 350 and name C)	(segid 3A4 and resid 382 and name CB)	6.34	0.61	0.60
	assign (segid 3A4 and resid 350 and name C)	(segid 3A4 and resid 382 and name N)	6.14	0.46	0.45
65	assign (segid 3A4 and resid 350 and name CA)	(segid 3A4 and resid 350 and name C)	1.53	0.01	0.01
	assign (segid 3A4 and resid 350 and name CA)	(segid 3A4 and resid 350 and name CB)	1.53	0.01	0.01
	assign (segid 3A4 and resid 350 and name CA)	(segid 3A4 and resid 350 and name O)	2.41	0.01	0.01
	assign (segid 3A4 and resid 350 and name CA)	(segid 3A4 and resid 351 and name C)	4.52	0.04	0.04
70	assign (segid 3A4 and resid 350 and name CA)	(segid 3A4 and resid 351 and name CA)	3.82	0.01	0.00
	assign (segid 3A4 and resid 350 and name CA)	(segid 3A4 and resid 351 and name N)	2.43	0.01	0.01
	assign (segid 3A4 and resid 350 and name CA)	(segid 3A4 and resid 351 and name O)	5.68	0.07	0.07
	assign (segid 3A4 and resid 350 and name CA)	(segid 3A4 and resid 352 and name C)	5.43	0.11	0.12
	assign (segid 3A4 and resid 350 and name CA)	(segid 3A4 and resid 352 and name CA)	5.39	0.08	0.08
75	assign (segid 3A4 and resid 350 and name CA)	(segid 3A4 and resid 352 and name CB)	6.04	0.13	0.13
	assign (segid 3A4 and resid 350 and name CA)	(segid 3A4 and resid 352 and name CG)	6.71	0.20	0.21
	assign (segid 3A4 and resid 350 and name CA)	(segid 3A4 and resid 352 and name N)	4.23	0.08	0.08
	assign (segid 3A4 and resid 350 and name CA)	(segid 3A4 and resid 352 and name O)	6.46	0.17	0.16
	assign (segid 3A4 and resid 350 and name CA)	(segid 3A4 and resid 353 and name C)	6.57	0.14	0.13
80	assign (segid 3A4 and resid 350 and name CA)	(segid 3A4 and resid 353 and name CA)	5.25	0.14	0.14
	assign (segid 3A4 and resid 350 and name CA)	(segid 3A4 and resid 353 and name CB)	4.61	0.19	0.19
	assign (segid 3A4 and resid 350 and name CA)	(segid 3A4 and resid 353 and name CG)	5.63	0.19	0.19
	assign (segid 3A4 and resid 350 and name CA)	(segid 3A4 and resid 353 and name N)	4.66	0.11	0.11
	assign (segid 3A4 and resid 350 and name CA)	(segid 3A4 and resid 353 and name O)	6.81	0.21	0.20

assign (segid 3A4 and resid 350 and name CA) (segid 3A4 and resid 353 and name OD1) 6.79 0.19 0.19
 assign (segid 3A4 and resid 350 and name CA) (segid 3A4 and resid 354 and name CA) 8.99 0.13 0.12
 assign (segid 3A4 and resid 350 and name CA) (segid 3A4 and resid 354 and name CB) 10.03 0.15 0.15
 assign (segid 3A4 and resid 350 and name CA) (segid 3A4 and resid 354 and name N) 7.65 0.13 0.13
 5 assign (segid 3A4 and resid 350 and name CA) (segid 3A4 and resid 355 and name CA) 9.73 0.37 0.36
 assign (segid 3A4 and resid 350 and name CA) (segid 3A4 and resid 355 and name CB) 9.64 0.49 0.50
 assign (segid 3A4 and resid 350 and name CA) (segid 3A4 and resid 356 and name CA) 8.42 0.50 0.49
 assign (segid 3A4 and resid 350 and name CA) (segid 3A4 and resid 356 and name CB) 7.14 0.57 0.56
 10 assign (segid 3A4 and resid 350 and name CA) (segid 3A4 and resid 357 and name CA) 9.36 0.25 0.25
 assign (segid 3A4 and resid 350 and name CA) (segid 3A4 and resid 357 and name CB) 8.60 0.19 0.19
 assign (segid 3A4 and resid 350 and name CA) (segid 3A4 and resid 358 and name CA) 12.57 0.40 0.39
 assign (segid 3A4 and resid 350 and name CA) (segid 3A4 and resid 358 and name CB) 13.88 0.39 0.39
 assign (segid 3A4 and resid 350 and name CA) (segid 3A4 and resid 359 and name CA) 13.37 0.36 0.35
 15 assign (segid 3A4 and resid 350 and name CA) (segid 3A4 and resid 359 and name CB) 14.70 0.26 0.26
 assign (segid 3A4 and resid 350 and name CA) (segid 3A4 and resid 360 and name CA) 10.04 0.24 0.25
 assign (segid 3A4 and resid 350 and name CA) (segid 3A4 and resid 360 and name CB) 8.87 0.33 0.33
 assign (segid 3A4 and resid 350 and name CA) (segid 3A4 and resid 361 and name CA) 12.11 0.19 0.20
 20 assign (segid 3A4 and resid 350 and name CA) (segid 3A4 and resid 361 and name CB) 12.72 0.25 0.25
 assign (segid 3A4 and resid 350 and name CA) (segid 3A4 and resid 362 and name CA) 14.75 0.17 0.17
 assign (segid 3A4 and resid 350 and name CA) (segid 3A4 and resid 362 and name CB) 15.52 0.21 0.21
 assign (segid 3A4 and resid 350 and name CA) (segid 3A4 and resid 363 and name CA) 15.44 0.21 0.20
 assign (segid 3A4 and resid 350 and name CA) (segid 3A4 and resid 363 and name CB) 16.19 0.31 0.31
 25 assign (segid 3A4 and resid 350 and name CA) (segid 3A4 and resid 364 and name CA) 16.80 0.11 0.10
 assign (segid 3A4 and resid 350 and name CA) (segid 3A4 and resid 364 and name CB) 16.69 0.12 0.12
 assign (segid 3A4 and resid 350 and name CA) (segid 3A4 and resid 365 and name CA) 17.86 0.36 0.37
 assign (segid 3A4 and resid 350 and name CA) (segid 3A4 and resid 365 and name CB) 19.09 0.34 0.34
 assign (segid 3A4 and resid 350 and name CA) (segid 3A4 and resid 381 and name CA) 7.32 0.64 0.64
 30 assign (segid 3A4 and resid 350 and name CA) (segid 3A4 and resid 382 and name CA) 7.07 0.53 0.54
 assign (segid 3A4 and resid 350 and name CA) (segid 3A4 and resid 382 and name CB) 6.24 0.58 0.58
 assign (segid 3A4 and resid 350 and name CA) (segid 3A4 and resid 382 and name N) 6.61 0.55 0.54
 assign (segid 3A4 and resid 350 and name CA) (segid 3A4 and resid 383 and name CA) 8.99 0.48 0.48
 assign (segid 3A4 and resid 350 and name CA) (segid 3A4 and resid 384 and name CA) 11.91 0.51 0.52
 35 assign (segid 3A4 and resid 350 and name CA) (segid 3A4 and resid 384 and name CB) 12.96 0.50 0.50
 assign (segid 3A4 and resid 350 and name CA) (segid 3A4 and resid 385 and name CA) 10.61 0.68 0.69
 assign (segid 3A4 and resid 350 and name CA) (segid 3A4 and resid 386 and name CA) 11.61 0.76 0.75
 assign (segid 3A4 and resid 350 and name CA) (segid 3A4 and resid 387 and name CA) 14.77 0.86 0.86
 assign (segid 3A4 and resid 350 and name CA) (segid 3A4 and resid 388 and name CA) 18.09 0.79 0.78
 40 assign (segid 3A4 and resid 350 and name CA) (segid 3A4 and resid 389 and name CA) 17.03 0.61 0.61
 assign (segid 3A4 and resid 350 and name CA) (segid 3A4 and resid 389 and name CB) 16.71 0.59 0.59
 assign (segid 3A4 and resid 350 and name CA) (segid 3A4 and resid 390 and name CA) 15.18 0.56 0.56
 assign (segid 3A4 and resid 350 and name CA) (segid 3A4 and resid 390 and name CB) 15.18 0.58 0.59
 assign (segid 3A4 and resid 350 and name CA) (segid 3A4 and resid 391 and name CA) 16.53 0.55 0.55
 45 assign (segid 3A4 and resid 350 and name CA) (segid 3A4 and resid 391 and name CB) 15.90 0.54 0.55
 assign (segid 3A4 and resid 350 and name CA) (segid 3A4 and resid 394 and name CA) 18.11 0.60 0.60
 assign (segid 3A4 and resid 350 and name CA) (segid 3A4 and resid 394 and name CB) 17.24 0.72 0.71
 assign (segid 3A4 and resid 350 and name CA) (segid 3A4 and resid 431 and name CA) 16.35 1.10 1.10
 50 assign (segid 3A4 and resid 350 and name CA) (segid 3A4 and resid 433 and name CA) 15.71 0.36 0.36
 assign (segid 3A4 and resid 350 and name CA) (segid 3A4 and resid 434 and name CA) 18.14 0.89 0.88
 assign (segid 3A4 and resid 350 and name CB) (segid 3A4 and resid 351 and name C) 5.48 0.06 0.06
 assign (segid 3A4 and resid 350 and name CB) (segid 3A4 and resid 351 and name CA) 4.42 0.07 0.07
 assign (segid 3A4 and resid 350 and name CB) (segid 3A4 and resid 351 and name N) 3.10 0.06 0.07
 55 assign (segid 3A4 and resid 350 and name CB) (segid 3A4 and resid 351 and name O) 6.58 0.09 0.09
 assign (segid 3A4 and resid 350 and name CB) (segid 3A4 and resid 352 and name C) 6.87 0.10 0.10
 assign (segid 3A4 and resid 350 and name CB) (segid 3A4 and resid 352 and name CA) 6.73 0.05 0.06
 assign (segid 3A4 and resid 350 and name CB) (segid 3A4 and resid 352 and name CB) 7.42 0.11 0.11
 60 assign (segid 3A4 and resid 350 and name CB) (segid 3A4 and resid 352 and name N) 5.47 0.05 0.05
 assign (segid 3A4 and resid 350 and name CB) (segid 3A4 and resid 353 and name CA) 6.57 0.15 0.15
 assign (segid 3A4 and resid 350 and name CB) (segid 3A4 and resid 353 and name CB) 5.74 0.20 0.20
 assign (segid 3A4 and resid 350 and name CB) (segid 3A4 and resid 353 and name CG) 6.62 0.21 0.22
 65 assign (segid 3A4 and resid 350 and name CB) (segid 3A4 and resid 353 and name N) 6.04 0.10 0.11
 assign (segid 3A4 and resid 350 and name CB) (segid 3A4 and resid 354 and name CA) 10.23 0.15 0.15
 assign (segid 3A4 and resid 350 and name CB) (segid 3A4 and resid 354 and name CB) 11.34 0.16 0.16
 assign (segid 3A4 and resid 350 and name CB) (segid 3A4 and resid 355 and name CA) 10.60 0.43 0.43
 70 assign (segid 3A4 and resid 350 and name CB) (segid 3A4 and resid 355 and name CB) 10.43 0.56 0.56
 assign (segid 3A4 and resid 350 and name CB) (segid 3A4 and resid 356 and name CA) 8.98 0.57 0.58
 assign (segid 3A4 and resid 350 and name CB) (segid 3A4 and resid 356 and name CB) 7.58 0.62 0.63
 assign (segid 3A4 and resid 350 and name CB) (segid 3A4 and resid 357 and name CA) 10.18 0.33 0.32
 75 assign (segid 3A4 and resid 350 and name CB) (segid 3A4 and resid 357 and name CB) 9.43 0.26 0.25
 assign (segid 3A4 and resid 350 and name CB) (segid 3A4 and resid 358 and name CA) 13.63 0.49 0.50
 assign (segid 3A4 and resid 350 and name CB) (segid 3A4 and resid 358 and name CB) 14.90 0.53 0.52
 assign (segid 3A4 and resid 350 and name CB) (segid 3A4 and resid 359 and name CA) 14.59 0.35 0.34
 80 assign (segid 3A4 and resid 350 and name CB) (segid 3A4 and resid 359 and name CB) 15.88 0.26 0.25
 assign (segid 3A4 and resid 350 and name CB) (segid 3A4 and resid 360 and name CA) 11.26 0.23 0.22
 assign (segid 3A4 and resid 350 and name CB) (segid 3A4 and resid 360 and name CB) 10.16 0.32 0.33
 assign (segid 3A4 and resid 350 and name CB) (segid 3A4 and resid 361 and name CA) 13.37 0.13 0.13
 assign (segid 3A4 and resid 350 and name CB) (segid 3A4 and resid 361 and name CB) 14.05 0.20 0.19
 assign (segid 3A4 and resid 350 and name CB) (segid 3A4 and resid 362 and name CA) 15.84 0.11 0.10
 assign (segid 3A4 and resid 350 and name CB) (segid 3A4 and resid 362 and name CB) 16.61 0.17 0.17
 assign (segid 3A4 and resid 350 and name CB) (segid 3A4 and resid 363 and name CA) 16.25 0.16 0.16
 80 assign (segid 3A4 and resid 350 and name CB) (segid 3A4 and resid 363 and name CB) 16.97 0.27 0.27
 assign (segid 3A4 and resid 350 and name CB) (segid 3A4 and resid 364 and name CA) 17.48 0.20 0.20
 assign (segid 3A4 and resid 350 and name CB) (segid 3A4 and resid 364 and name CB) 17.43 0.22 0.23
 assign (segid 3A4 and resid 350 and name CB) (segid 3A4 and resid 365 and name CA) 18.25 0.42 0.42

	assign (segid 3A4 and resid 350 and name CB)	(segid 3A4 and resid 381 and name C)	6.56	0.74	0.74
	assign (segid 3A4 and resid 350 and name CB)	(segid 3A4 and resid 381 and name CA)	6.71	0.73	0.74
	assign (segid 3A4 and resid 350 and name CB)	(segid 3A4 and resid 382 and name C)	6.53	0.51	0.51
	assign (segid 3A4 and resid 350 and name CB)	(segid 3A4 and resid 382 and name CA)	5.93	0.54	0.54
5	assign (segid 3A4 and resid 350 and name CB)	(segid 3A4 and resid 382 and name CB)	4.94	0.55	0.55
	assign (segid 3A4 and resid 350 and name CB)	(segid 3A4 and resid 382 and name N)	5.66	0.60	0.61
	assign (segid 3A4 and resid 350 and name CB)	(segid 3A4 and resid 382 and name O)	6.60	0.47	0.47
	assign (segid 3A4 and resid 350 and name CB)	(segid 3A4 and resid 383 and name CA)	8.20	0.46	0.46
	assign (segid 3A4 and resid 350 and name CB)	(segid 3A4 and resid 384 and name CA)	10.81	0.50	0.51
10	assign (segid 3A4 and resid 350 and name CB)	(segid 3A4 and resid 384 and name CB)	11.86	0.51	0.51
	assign (segid 3A4 and resid 350 and name CB)	(segid 3A4 and resid 385 and name CA)	9.27	0.66	0.67
	assign (segid 3A4 and resid 350 and name CB)	(segid 3A4 and resid 386 and name CA)	10.13	0.75	0.74
	assign (segid 3A4 and resid 350 and name CB)	(segid 3A4 and resid 387 and name CA)	13.29	0.86	0.85
	assign (segid 3A4 and resid 350 and name CB)	(segid 3A4 and resid 388 and name CA)	16.60	0.77	0.77
15	assign (segid 3A4 and resid 350 and name CB)	(segid 3A4 and resid 388 and name CB)	17.62	0.85	0.85
	assign (segid 3A4 and resid 350 and name CB)	(segid 3A4 and resid 389 and name CA)	15.60	0.57	0.57
	assign (segid 3A4 and resid 350 and name CB)	(segid 3A4 and resid 389 and name CB)	15.31	0.55	0.54
	assign (segid 3A4 and resid 350 and name CB)	(segid 3A4 and resid 390 and name CA)	13.77	0.55	0.56
	assign (segid 3A4 and resid 350 and name CB)	(segid 3A4 and resid 390 and name CB)	13.76	0.60	0.60
20	assign (segid 3A4 and resid 350 and name CB)	(segid 3A4 and resid 391 and name CA)	15.28	0.53	0.53
	assign (segid 3A4 and resid 350 and name CB)	(segid 3A4 and resid 391 and name CB)	14.73	0.54	0.53
	assign (segid 3A4 and resid 350 and name CB)	(segid 3A4 and resid 392 and name CA)	18.91	0.56	0.56
	assign (segid 3A4 and resid 350 and name CB)	(segid 3A4 and resid 394 and name CA)	17.07	0.63	0.63
	assign (segid 3A4 and resid 350 and name CB)	(segid 3A4 and resid 394 and name CB)	16.15	0.76	0.75
25	assign (segid 3A4 and resid 350 and name CB)	(segid 3A4 and resid 397 and name CB)	18.18	0.52	0.52
	assign (segid 3A4 and resid 350 and name CB)	(segid 3A4 and resid 430 and name CA)	17.29	1.85	1.85
	assign (segid 3A4 and resid 350 and name CB)	(segid 3A4 and resid 431 and name CA)	16.12	1.12	1.11
	assign (segid 3A4 and resid 350 and name CB)	(segid 3A4 and resid 433 and name CA)	15.84	0.28	0.27
30	assign (segid 3A4 and resid 350 and name CB)	(segid 3A4 and resid 434 and name CA)	18.32	0.91	0.91
	assign (segid 3A4 and resid 350 and name N)	(segid 3A4 and resid 350 and name C)	2.46	0.01	0.02
	assign (segid 3A4 and resid 350 and name N)	(segid 3A4 and resid 350 and name CA)	1.45	0.02	0.01
	assign (segid 3A4 and resid 350 and name N)	(segid 3A4 and resid 350 and name CB)	2.46	0.03	0.04
	assign (segid 3A4 and resid 350 and name N)	(segid 3A4 and resid 350 and name O)	3.52	0.03	0.03
35	assign (segid 3A4 and resid 350 and name N)	(segid 3A4 and resid 351 and name C)	4.77	0.03	0.03
	assign (segid 3A4 and resid 350 and name N)	(segid 3A4 and resid 351 and name CA)	4.22	0.03	0.02
	assign (segid 3A4 and resid 350 and name N)	(segid 3A4 and resid 351 and name N)	2.81	0.03	0.02
	assign (segid 3A4 and resid 350 and name N)	(segid 3A4 and resid 351 and name O)	6.00	0.04	0.04
	assign (segid 3A4 and resid 350 and name N)	(segid 3A4 and resid 352 and name C)	5.51	0.09	0.09
40	assign (segid 3A4 and resid 350 and name N)	(segid 3A4 and resid 352 and name CA)	5.30	0.06	0.06
	assign (segid 3A4 and resid 350 and name N)	(segid 3A4 and resid 352 and name CB)	5.59	0.14	0.13
	assign (segid 3A4 and resid 350 and name N)	(segid 3A4 and resid 352 and name CG)	6.15	0.25	0.26
	assign (segid 3A4 and resid 350 and name N)	(segid 3A4 and resid 352 and name N)	1.24	0.04	0.04
	assign (segid 3A4 and resid 350 and name N)	(segid 3A4 and resid 352 and name O)	6.43	0.15	0.15
45	assign (segid 3A4 and resid 350 and name N)	(segid 3A4 and resid 353 and name C)	7.16	0.15	0.14
	assign (segid 3A4 and resid 350 and name N)	(segid 3A4 and resid 353 and name CA)	5.74	0.15	0.14
	assign (segid 3A4 and resid 350 and name N)	(segid 3A4 and resid 353 and name CB)	5.38	0.20	0.20
	assign (segid 3A4 and resid 350 and name N)	(segid 3A4 and resid 353 and name CG)	6.40	0.20	0.20
	assign (segid 3A4 and resid 350 and name N)	(segid 3A4 and resid 353 and name N)	5.03	0.11	0.12
	assign (segid 3A4 and resid 350 and name N)	(segid 3A4 and resid 353 and name O)	7.57	0.20	0.20
50	assign (segid 3A4 and resid 350 and name N)	(segid 3A4 and resid 353 and name OD1)	7.50	0.20	0.19
	assign (segid 3A4 and resid 350 and name O)	(segid 3A4 and resid 350 and name CB)	3.26	0.03	0.03
	assign (segid 3A4 and resid 350 and name O)	(segid 3A4 and resid 351 and name C)	3.15	0.06	0.06
	assign (segid 3A4 and resid 350 and name O)	(segid 3A4 and resid 351 and name CA)	2.77	0.05	0.04
	assign (segid 3A4 and resid 350 and name O)	(segid 3A4 and resid 351 and name N)	2.24	0.02	0.02
55	assign (segid 3A4 and resid 350 and name O)	(segid 3A4 and resid 351 and name O)	4.03	0.12	0.13
	assign (segid 3A4 and resid 350 and name O)	(segid 3A4 and resid 352 and name C)	4.26	0.13	0.12
	assign (segid 3A4 and resid 350 and name O)	(segid 3A4 and resid 352 and name CA)	4.31	0.12	0.13
	assign (segid 3A4 and resid 350 and name O)	(segid 3A4 and resid 352 and name CB)	5.48	0.11	0.12
	assign (segid 3A4 and resid 350 and name O)	(segid 3A4 and resid 352 and name CG)	6.25	0.15	0.15
60	assign (segid 3A4 and resid 350 and name O)	(segid 3A4 and resid 352 and name N)	3.24	0.11	0.11
	assign (segid 3A4 and resid 350 and name O)	(segid 3A4 and resid 352 and name O)	5.40	0.13	0.13
	assign (segid 3A4 and resid 350 and name O)	(segid 3A4 and resid 353 and name C)	4.92	0.16	0.17
	assign (segid 3A4 and resid 350 and name O)	(segid 3A4 and resid 353 and name CA)	3.96	0.11	0.11
	assign (segid 3A4 and resid 350 and name O)	(segid 3A4 and resid 353 and name CB)	3.42	0.14	0.14
65	assign (segid 3A4 and resid 350 and name O)	(segid 3A4 and resid 353 and name CG)	4.74	0.14	0.14
	assign (segid 3A4 and resid 350 and name O)	(segid 3A4 and resid 353 and name N)	3.28	0.11	0.11
	assign (segid 3A4 and resid 350 and name O)	(segid 3A4 and resid 353 and name O)	4.84	0.26	0.26
	assign (segid 3A4 and resid 350 and name O)	(segid 3A4 and resid 353 and name OD1)	5.79	0.16	0.16
	assign (segid 3A4 and resid 350 and name O)	(segid 3A4 and resid 354 and name CA)	7.34	0.17	0.17
70	assign (segid 3A4 and resid 350 and name O)	(segid 3A4 and resid 354 and name N)	6.18	0.15	0.14
	assign (segid 3A4 and resid 350 and name O)	(segid 3A4 and resid 355 and name N)	7.41	0.30	0.31
	assign (segid 3A4 and resid 350 and name O)	(segid 3A4 and resid 356 and name C)	6.65	0.46	0.45
	assign (segid 3A4 and resid 350 and name O)	(segid 3A4 and resid 356 and name CA)	6.30	0.52	0.52
	assign (segid 3A4 and resid 350 and name O)	(segid 3A4 and resid 356 and name CB)	5.06	0.59	0.59
75	assign (segid 3A4 and resid 350 and name O)	(segid 3A4 and resid 356 and name N)	6.45	0.44	0.43
	assign (segid 3A4 and resid 350 and name O)	(segid 3A4 and resid 357 and name CA)	7.01	0.26	0.26
	assign (segid 3A4 and resid 350 and name O)	(segid 3A4 and resid 357 and name CB)	6.28	0.18	0.18
	assign (segid 3A4 and resid 350 and name O)	(segid 3A4 and resid 357 and name N)	6.30	0.36	0.36
	assign (segid 3A4 and resid 350 and name O)	(segid 3A4 and resid 381 and name C)	6.93	0.43	0.44
80	assign (segid 3A4 and resid 350 and name O)	(segid 3A4 and resid 381 and name CA)	6.36	0.41	0.42
	assign (segid 3A4 and resid 350 and name O)	(segid 3A4 and resid 381 and name N)	6.70	0.62	0.62
	assign (segid 3A4 and resid 350 and name O)	(segid 3A4 and resid 382 and name N)	6.46	0.41	0.42
	assign (segid 3A4 and resid 351 and name C)	(segid 3A4 and resid 351 and name O)	1.24	0.02	0.01

	assign (segid 3A4 and resid 351 and name C) (segid 3A4 and resid 352 and name C)	3.45	0.07	0.07
	assign (segid 3A4 and resid 351 and name C) (segid 3A4 and resid 352 and name CA)	2.14	0.02	0.01
	assign (segid 3A4 and resid 351 and name C) (segid 3A4 and resid 352 and name CB)	3.52	0.07	0.07
	assign (segid 3A4 and resid 351 and name C) (segid 3A4 and resid 352 and name CG)	3.75	0.19	0.20
5	assign (segid 3A4 and resid 351 and name C) (segid 3A4 and resid 352 and name N)	1.32	0.01	0.02
	assign (segid 3A4 and resid 351 and name C) (segid 3A4 and resid 352 and name O)	4.60	0.08	0.08
	assign (segid 3A4 and resid 351 and name C) (segid 3A4 and resid 353 and name C)	5.50	0.22	0.21
	assign (segid 3A4 and resid 351 and name C) (segid 3A4 and resid 353 and name CA)	4.87	0.12	0.11
	assign (segid 3A4 and resid 351 and name C) (segid 3A4 and resid 353 and name CB)	5.30	0.13	0.14
10	assign (segid 3A4 and resid 351 and name C) (segid 3A4 and resid 353 and name CG)	6.83	0.15	0.14
	assign (segid 3A4 and resid 351 and name C) (segid 3A4 and resid 353 and name N)	3.48	0.08	0.09
	assign (segid 3A4 and resid 351 and name C) (segid 3A4 and resid 353 and name O)	5.41	0.29	0.29
	assign (segid 3A4 and resid 351 and name C) (segid 3A4 and resid 353 and name OD1)	7.56	0.16	0.15
	assign (segid 3A4 and resid 351 and name C) (segid 3A4 and resid 354 and name CA)	7.53	0.22	0.21
15	assign (segid 3A4 and resid 351 and name C) (segid 3A4 and resid 354 and name N)	6.55	0.19	0.20
	assign (segid 3A4 and resid 351 and name C) (segid 3A4 and resid 356 and name C)	7.31	0.45	0.46
	assign (segid 3A4 and resid 351 and name C) (segid 3A4 and resid 356 and name CB)	6.73	0.54	0.54
	assign (segid 3A4 and resid 351 and name C) (segid 3A4 and resid 357 and name C)	7.34	0.36	0.36
	assign (segid 3A4 and resid 351 and name C) (segid 3A4 and resid 357 and name CA)	6.58	0.31	0.31
20	assign (segid 3A4 and resid 351 and name C) (segid 3A4 and resid 357 and name CB)	5.34	0.26	0.26
	assign (segid 3A4 and resid 351 and name C) (segid 3A4 and resid 357 and name N)	6.52	0.39	0.38
	assign (segid 3A4 and resid 351 and name C) (segid 3A4 and resid 360 and name C)	6.38	0.14	0.15
	assign (segid 3A4 and resid 351 and name C) (segid 3A4 and resid 360 and name CA)	6.09	0.19	0.19
	assign (segid 3A4 and resid 351 and name C) (segid 3A4 and resid 360 and name CB)	5.30	0.28	0.28
25	assign (segid 3A4 and resid 351 and name C) (segid 3A4 and resid 360 and name N)	7.37	0.23	0.23
	assign (segid 3A4 and resid 351 and name C) (segid 3A4 and resid 360 and name O)	5.89	0.12	0.12
	assign (segid 3A4 and resid 351 and name C) (segid 3A4 and resid 361 and name N)	7.49	0.16	0.15
	assign (segid 3A4 and resid 351 and name C) (segid 3A4 and resid 381 and name CA)	6.71	0.55	0.54
	assign (segid 3A4 and resid 351 and name CA) (segid 3A4 and resid 351 and name C)	1.54	0.02	0.01
30	assign (segid 3A4 and resid 351 and name CA) (segid 3A4 and resid 351 and name O)	2.40	0.01	0.01
	assign (segid 3A4 and resid 351 and name CA) (segid 3A4 and resid 352 and name C)	4.70	0.04	0.04
	assign (segid 3A4 and resid 351 and name CA) (segid 3A4 and resid 352 and name CA)	3.82	0.01	0.02
	assign (segid 3A4 and resid 351 and name CA) (segid 3A4 and resid 352 and name CB)	4.75	0.06	0.07
	assign (segid 3A4 and resid 351 and name CA) (segid 3A4 and resid 352 and name CG)	4.87	0.18	0.17
35	assign (segid 3A4 and resid 351 and name CA) (segid 3A4 and resid 352 and name N)	2.45	0.01	0.01
	assign (segid 3A4 and resid 351 and name CA) (segid 3A4 and resid 352 and name O)	5.90	0.04	0.05
	assign (segid 3A4 and resid 351 and name CA) (segid 3A4 and resid 353 and name C)	6.46	0.23	0.22
	assign (segid 3A4 and resid 351 and name CA) (segid 3A4 and resid 353 and name CA)	5.68	0.10	0.11
	assign (segid 3A4 and resid 351 and name CA) (segid 3A4 and resid 353 and name CB)	5.74	0.13	0.14
40	assign (segid 3A4 and resid 351 and name CA) (segid 3A4 and resid 353 and name CG)	7.21	0.14	0.15
	assign (segid 3A4 and resid 351 and name CA) (segid 3A4 and resid 353 and name N)	4.44	0.07	0.06
	assign (segid 3A4 and resid 351 and name CA) (segid 3A4 and resid 353 and name O)	6.29	0.32	0.33
	assign (segid 3A4 and resid 351 and name CA) (segid 3A4 and resid 354 and name CA)	8.65	0.25	0.25
	assign (segid 3A4 and resid 351 and name CA) (segid 3A4 and resid 354 and name CB)	9.85	0.20	0.20
45	assign (segid 3A4 and resid 351 and name CA) (segid 3A4 and resid 354 and name N)	7.62	0.21	0.21
	assign (segid 3A4 and resid 351 and name CA) (segid 3A4 and resid 355 and name CA)	10.11	0.42	0.43
	assign (segid 3A4 and resid 351 and name CA) (segid 3A4 and resid 355 and name CB)	10.58	0.49	0.49
	assign (segid 3A4 and resid 351 and name CA) (segid 3A4 and resid 356 and name CA)	7.95	0.60	0.61
	assign (segid 3A4 and resid 351 and name CA) (segid 3A4 and resid 356 and name CB)	6.86	0.67	0.67
50	assign (segid 3A4 and resid 351 and name CA) (segid 3A4 and resid 357 and name CA)	7.41	0.42	0.43
	assign (segid 3A4 and resid 351 and name CA) (segid 3A4 and resid 357 and name CB)	6.21	0.37	0.38
	assign (segid 3A4 and resid 351 and name CA) (segid 3A4 and resid 357 and name N)	7.23	0.50	0.50
	assign (segid 3A4 and resid 351 and name CA) (segid 3A4 and resid 358 and name CA)	10.75	0.50	0.50
	assign (segid 3A4 and resid 351 and name CA) (segid 3A4 and resid 358 and name CB)	12.04	0.52	0.53
55	assign (segid 3A4 and resid 351 and name CA) (segid 3A4 and resid 359 and name CA)	11.12	0.28	0.29
	assign (segid 3A4 and resid 351 and name CA) (segid 3A4 and resid 359 and name CB)	12.27	0.27	0.26
	assign (segid 3A4 and resid 351 and name CA) (segid 3A4 and resid 360 and name CA)	7.55	0.21	0.20
	assign (segid 3A4 and resid 351 and name CA) (segid 3A4 and resid 360 and name CB)	6.80	0.29	0.29
	assign (segid 3A4 and resid 351 and name CA) (segid 3A4 and resid 360 and name O)	7.23	0.14	0.14
60	assign (segid 3A4 and resid 351 and name CA) (segid 3A4 and resid 361 and name CA)	9.57	0.14	0.15
	assign (segid 3A4 and resid 351 and name CA) (segid 3A4 and resid 361 and name CB)	10.51	0.18	0.17
	assign (segid 3A4 and resid 351 and name CA) (segid 3A4 and resid 362 and name CA)	11.65	0.11	0.10
	assign (segid 3A4 and resid 351 and name CA) (segid 3A4 and resid 362 and name CB)	12.47	0.15	0.16
	assign (segid 3A4 and resid 351 and name CA) (segid 3A4 and resid 363 and name CA)	11.88	0.17	0.16
65	assign (segid 3A4 and resid 351 and name CA) (segid 3A4 and resid 363 and name CB)	12.63	0.26	0.25
	assign (segid 3A4 and resid 351 and name CA) (segid 3A4 and resid 364 and name CA)	13.18	0.14	0.14
	assign (segid 3A4 and resid 351 and name CA) (segid 3A4 and resid 364 and name CB)	13.19	0.20	0.20
	assign (segid 3A4 and resid 351 and name CA) (segid 3A4 and resid 365 and name CA)	14.18	0.26	0.26
	assign (segid 3A4 and resid 351 and name CA) (segid 3A4 and resid 365 and name CB)	15.38	0.25	0.26
70	assign (segid 3A4 and resid 351 and name CA) (segid 3A4 and resid 381 and name C)	6.21	0.53	0.53
	assign (segid 3A4 and resid 351 and name CA) (segid 3A4 and resid 381 and name CA)	5.55	0.62	0.61
	assign (segid 3A4 and resid 351 and name CA) (segid 3A4 and resid 381 and name N)	6.27	0.65	0.65
	assign (segid 3A4 and resid 351 and name CA) (segid 3A4 and resid 382 and name CA)	6.70	0.54	0.54
	assign (segid 3A4 and resid 351 and name CA) (segid 3A4 and resid 382 and name CB)	6.69	0.67	0.67
75	assign (segid 3A4 and resid 351 and name CA) (segid 3A4 and resid 382 and name N)	5.69	0.48	0.48
	assign (segid 3A4 and resid 351 and name CA) (segid 3A4 and resid 383 and name CA)	7.68	0.51	0.51
	assign (segid 3A4 and resid 351 and name CA) (segid 3A4 and resid 384 and name CA)	11.17	0.53	0.53
	assign (segid 3A4 and resid 351 and name CA) (segid 3A4 and resid 384 and name CB)	12.00	0.50	0.50
	assign (segid 3A4 and resid 351 and name CA) (segid 3A4 and resid 385 and name CA)	11.10	0.70	0.70
80	assign (segid 3A4 and resid 351 and name CA) (segid 3A4 and resid 386 and name CA)	12.60	0.71	0.71
	assign (segid 3A4 and resid 351 and name CA) (segid 3A4 and resid 387 and name CA)	16.09	0.69	0.68
	assign (segid 3A4 and resid 351 and name CA) (segid 3A4 and resid 389 and name CA)	18.06	0.58	0.58
	assign (segid 3A4 and resid 351 and name CA) (segid 3A4 and resid 389 and name CB)	17.95	0.60	0.60

	assign	(segid 3A4 and resid 351 and name CA)	(segid 3A4 and resid 390 and name CA)	15.56	0.50	0.50
	assign	(segid 3A4 and resid 351 and name CA)	(segid 3A4 and resid 390 and name CB)	15.45	0.47	0.47
	assign	(segid 3A4 and resid 351 and name CA)	(segid 3A4 and resid 391 and name CA)	16.23	0.54	0.53
	assign	(segid 3A4 and resid 351 and name CA)	(segid 3A4 and resid 391 and name CB)	15.32	0.50	0.51
5	assign	(segid 3A4 and resid 351 and name CA)	(segid 3A4 and resid 394 and name CA)	16.70	0.53	0.53
	assign	(segid 3A4 and resid 351 and name CA)	(segid 3A4 and resid 394 and name CB)	15.95	0.60	0.60
	assign	(segid 3A4 and resid 351 and name CA)	(segid 3A4 and resid 397 and name CA)	18.25	0.50	0.51
	assign	(segid 3A4 and resid 351 and name CA)	(segid 3A4 and resid 397 and name CB)	17.04	0.50	0.51
	assign	(segid 3A4 and resid 351 and name CA)	(segid 3A4 and resid 398 and name CA)	17.40	0.55	0.55
10	assign	(segid 3A4 and resid 351 and name CA)	(segid 3A4 and resid 398 and name CB)	16.96	0.53	0.54
	assign	(segid 3A4 and resid 351 and name CA)	(segid 3A4 and resid 429 and name CA)	18.11	0.43	0.44
	assign	(segid 3A4 and resid 351 and name CA)	(segid 3A4 and resid 431 and name CA)	16.68	1.04	1.03
	assign	(segid 3A4 and resid 351 and name CA)	(segid 3A4 and resid 433 and name CA)	14.66	0.62	0.62
	assign	(segid 3A4 and resid 351 and name CA)	(segid 3A4 and resid 434 and name CA)	16.50	0.95	0.94
15	assign	(segid 3A4 and resid 351 and name CA)	(segid 3A4 and resid 435 and name CA)	18.69	0.91	0.91
	assign	(segid 3A4 and resid 351 and name N)	(segid 3A4 and resid 351 and name C)	2.50	0.02	0.01
	assign	(segid 3A4 and resid 351 and name N)	(segid 3A4 and resid 351 and name CA)	1.46	0.00	0.01
	assign	(segid 3A4 and resid 351 and name N)	(segid 3A4 and resid 351 and name O)	3.63	0.03	0.02
	assign	(segid 3A4 and resid 351 and name N)	(segid 3A4 and resid 352 and name C)	4.82	0.03	0.03
20	assign	(segid 3A4 and resid 351 and name N)	(segid 3A4 and resid 352 and name CA)	4.18	0.02	0.03
	assign	(segid 3A4 and resid 351 and name N)	(segid 3A4 and resid 352 and name CB)	4.95	0.07	0.06
	assign	(segid 3A4 and resid 351 and name N)	(segid 3A4 and resid 352 and name CG)	5.25	0.16	0.15
	assign	(segid 3A4 and resid 351 and name N)	(segid 3A4 and resid 352 and name N)	2.74	0.03	0.04
	assign	(segid 3A4 and resid 351 and name N)	(segid 3A4 and resid 352 and name O)	6.01	0.05	0.04
25	assign	(segid 3A4 and resid 351 and name N)	(segid 3A4 and resid 353 and name C)	6.54	0.16	0.16
	assign	(segid 3A4 and resid 351 and name N)	(segid 3A4 and resid 353 and name CA)	5.50	0.08	0.08
	assign	(segid 3A4 and resid 351 and name N)	(segid 3A4 and resid 353 and name CB)	5.33	0.14	0.15
	assign	(segid 3A4 and resid 351 and name N)	(segid 3A4 and resid 353 and name CG)	6.71	0.14	0.14
30	assign	(segid 3A4 and resid 351 and name N)	(segid 3A4 and resid 353 and name N)	4.39	0.06	0.07
	assign	(segid 3A4 and resid 351 and name N)	(segid 3A4 and resid 353 and name O)	6.56	0.26	0.26
	assign	(segid 3A4 and resid 351 and name N)	(segid 3A4 and resid 354 and name N)	7.70	0.12	0.12
	assign	(segid 3A4 and resid 351 and name N)	(segid 3A4 and resid 356 and name CB)	7.08	0.62	0.63
	assign	(segid 3A4 and resid 351 and name N)	(segid 3A4 and resid 357 and name CB)	7.25	0.28	0.27
35	assign	(segid 3A4 and resid 351 and name N)	(segid 3A4 and resid 381 and name C)	6.42	0.59	0.60
	assign	(segid 3A4 and resid 351 and name N)	(segid 3A4 and resid 381 and name CA)	6.03	0.67	0.68
	assign	(segid 3A4 and resid 351 and name N)	(segid 3A4 and resid 381 and name N)	6.76	0.72	0.72
	assign	(segid 3A4 and resid 351 and name N)	(segid 3A4 and resid 382 and name CA)	6.48	0.53	0.52
	assign	(segid 3A4 and resid 351 and name N)	(segid 3A4 and resid 382 and name CB)	6.16	0.63	0.62
40	assign	(segid 3A4 and resid 351 and name N)	(segid 3A4 and resid 382 and name N)	5.70	0.52	0.51
	assign	(segid 3A4 and resid 351 and name O)	(segid 3A4 and resid 352 and name C)	3.79	0.11	0.11
	assign	(segid 3A4 and resid 351 and name O)	(segid 3A4 and resid 352 and name CA)	2.77	0.03	0.04
	assign	(segid 3A4 and resid 351 and name O)	(segid 3A4 and resid 352 and name CB)	3.90	0.13	0.12
	assign	(segid 3A4 and resid 351 and name O)	(segid 3A4 and resid 352 and name CG)	3.97	0.31	0.32
45	assign	(segid 3A4 and resid 351 and name O)	(segid 3A4 and resid 352 and name N)	2.25	0.01	0.00
	assign	(segid 3A4 and resid 351 and name O)	(segid 3A4 and resid 352 and name O)	4.82	0.15	0.14
	assign	(segid 3A4 and resid 351 and name O)	(segid 3A4 and resid 353 and name C)	5.61	0.28	0.28
	assign	(segid 3A4 and resid 351 and name O)	(segid 3A4 and resid 353 and name CA)	5.31	0.18	0.17
	assign	(segid 3A4 and resid 351 and name O)	(segid 3A4 and resid 353 and name CB)	5.88	0.18	0.18
50	assign	(segid 3A4 and resid 351 and name O)	(segid 3A4 and resid 353 and name CG)	7.38	0.20	0.20
	assign	(segid 3A4 and resid 351 and name O)	(segid 3A4 and resid 353 and name N)	3.97	0.12	0.13
	assign	(segid 3A4 and resid 351 and name O)	(segid 3A4 and resid 353 and name O)	5.35	0.36	0.37
	assign	(segid 3A4 and resid 351 and name O)	(segid 3A4 and resid 354 and name CA)	7.38	0.31	0.31
	assign	(segid 3A4 and resid 351 and name O)	(segid 3A4 and resid 354 and name N)	6.61	0.28	0.28
	assign	(segid 3A4 and resid 351 and name O)	(segid 3A4 and resid 356 and name C)	6.89	0.48	0.49
55	assign	(segid 3A4 and resid 351 and name O)	(segid 3A4 and resid 356 and name CB)	6.71	0.53	0.54
	assign	(segid 3A4 and resid 351 and name O)	(segid 3A4 and resid 357 and name C)	6.56	0.41	0.41
	assign	(segid 3A4 and resid 351 and name O)	(segid 3A4 and resid 357 and name CA)	5.83	0.36	0.36
	assign	(segid 3A4 and resid 351 and name O)	(segid 3A4 and resid 357 and name CB)	4.46	0.31	0.31
	assign	(segid 3A4 and resid 351 and name O)	(segid 3A4 and resid 357 and name N)	6.01	0.43	0.43
60	assign	(segid 3A4 and resid 351 and name O)	(segid 3A4 and resid 357 and name O)	6.39	0.61	0.61
	assign	(segid 3A4 and resid 351 and name O)	(segid 3A4 and resid 359 and name C)	7.53	0.25	0.25
	assign	(segid 3A4 and resid 351 and name O)	(segid 3A4 and resid 360 and name C)	5.53	0.18	0.19
	assign	(segid 3A4 and resid 351 and name O)	(segid 3A4 and resid 360 and name CA)	5.21	0.21	0.22
	assign	(segid 3A4 and resid 351 and name O)	(segid 3A4 and resid 360 and name CB)	4.66	0.32	0.31
65	assign	(segid 3A4 and resid 351 and name O)	(segid 3A4 and resid 360 and name N)	6.52	0.25	0.25
	assign	(segid 3A4 and resid 351 and name O)	(segid 3A4 and resid 360 and name O)	5.00	0.16	0.16
	assign	(segid 3A4 and resid 351 and name O)	(segid 3A4 and resid 361 and name CA)	7.47	0.19	0.19
	assign	(segid 3A4 and resid 351 and name O)	(segid 3A4 and resid 361 and name N)	6.73	0.19	0.19
	assign	(segid 3A4 and resid 351 and name O)	(segid 3A4 and resid 381 and name CA)	6.79	0.49	0.49
70	assign	(segid 3A4 and resid 352 and name C)	(segid 3A4 and resid 352 and name CB)	2.51	0.02	0.02
	assign	(segid 3A4 and resid 352 and name C)	(segid 3A4 and resid 352 and name CG)	3.89	0.05	0.04
	assign	(segid 3A4 and resid 352 and name C)	(segid 3A4 and resid 352 and name O)	1.23	0.00	0.01
	assign	(segid 3A4 and resid 352 and name C)	(segid 3A4 and resid 353 and name C)	3.07	0.05	0.06
	assign	(segid 3A4 and resid 352 and name C)	(segid 3A4 and resid 353 and name CA)	2.44	0.01	0.02
75	assign	(segid 3A4 and resid 352 and name C)	(segid 3A4 and resid 353 and name CB)	3.71	0.03	0.03
	assign	(segid 3A4 and resid 352 and name C)	(segid 3A4 and resid 353 and name CG)	4.97	0.05	0.06
	assign	(segid 3A4 and resid 352 and name C)	(segid 3A4 and resid 353 and name N)	1.34	0.01	0.01
	assign	(segid 3A4 and resid 352 and name C)	(segid 3A4 and resid 353 and name O)	3.68	0.14	0.14
	assign	(segid 3A4 and resid 352 and name C)	(segid 3A4 and resid 353 and name OD1)	5.32	0.10	0.10
80	assign	(segid 3A4 and resid 352 and name C)	(segid 3A4 and resid 354 and name C)	5.94	0.05	0.05
	assign	(segid 3A4 and resid 352 and name C)	(segid 3A4 and resid 354 and name CA)	4.83	0.07	0.07
	assign	(segid 3A4 and resid 352 and name C)	(segid 3A4 and resid 354 and name CB)	5.66	0.10	0.11
	assign	(segid 3A4 and resid 352 and name C)	(segid 3A4 and resid 354 and name N)	3.69	0.06	0.06

	assign	(segid 3A4 and resid 352 and name C)	(segid 3A4 and resid 354 and name O)	6.78	0.10	0.11
	assign	(segid 3A4 and resid 352 and name C)	(segid 3A4 and resid 355 and name C)	7.59	0.07	0.07
	assign	(segid 3A4 and resid 352 and name C)	(segid 3A4 and resid 355 and name CA)	7.48	0.08	0.09
5	assign	(segid 3A4 and resid 352 and name C)	(segid 3A4 and resid 355 and name N)	6.23	0.07	0.07
	assign	(segid 3A4 and resid 352 and name C)	(segid 3A4 and resid 356 and name C)	7.00	0.11	0.11
	assign	(segid 3A4 and resid 352 and name C)	(segid 3A4 and resid 356 and name CA)	7.08	0.14	0.14
	assign	(segid 3A4 and resid 352 and name C)	(segid 3A4 and resid 356 and name CB)	6.66	0.24	0.25
	assign	(segid 3A4 and resid 352 and name C)	(segid 3A4 and resid 356 and name N)	6.61	0.10	0.11
10	assign	(segid 3A4 and resid 352 and name C)	(segid 3A4 and resid 357 and name C)	6.49	0.29	0.29
	assign	(segid 3A4 and resid 352 and name C)	(segid 3A4 and resid 357 and name CA)	6.29	0.13	0.13
	assign	(segid 3A4 and resid 352 and name C)	(segid 3A4 and resid 357 and name CB)	5.54	0.15	0.16
	assign	(segid 3A4 and resid 352 and name C)	(segid 3A4 and resid 357 and name N)	5.98	0.09	0.10
	assign	(segid 3A4 and resid 352 and name C)	(segid 3A4 and resid 360 and name C)	5.79	0.25	0.25
15	assign	(segid 3A4 and resid 352 and name C)	(segid 3A4 and resid 360 and name CA)	5.19	0.27	0.27
	assign	(segid 3A4 and resid 352 and name C)	(segid 3A4 and resid 360 and name CB)	3.78	0.31	0.31
	assign	(segid 3A4 and resid 352 and name C)	(segid 3A4 and resid 360 and name N)	6.06	0.34	0.34
	assign	(segid 3A4 and resid 352 and name C)	(segid 3A4 and resid 360 and name O)	5.94	0.19	0.19
	assign	(segid 3A4 and resid 352 and name C)	(segid 3A4 and resid 361 and name N)	6.53	0.30	0.30
20	assign	(segid 3A4 and resid 352 and name CA)	(segid 3A4 and resid 352 and name C)	1.53	0.01	0.01
	assign	(segid 3A4 and resid 352 and name CA)	(segid 3A4 and resid 352 and name CB)	1.53	0.01	0.01
	assign	(segid 3A4 and resid 352 and name CA)	(segid 3A4 and resid 352 and name CG)	2.57	0.04	0.04
	assign	(segid 3A4 and resid 352 and name CA)	(segid 3A4 and resid 352 and name O)	2.42	0.01	0.00
	assign	(segid 3A4 and resid 352 and name CA)	(segid 3A4 and resid 353 and name C)	4.44	0.05	0.04
25	assign	(segid 3A4 and resid 352 and name CA)	(segid 3A4 and resid 353 and name CA)	3.82	0.02	0.02
	assign	(segid 3A4 and resid 352 and name CA)	(segid 3A4 and resid 353 and name CB)	4.86	0.04	0.04
	assign	(segid 3A4 and resid 352 and name CA)	(segid 3A4 and resid 353 and name CG)	6.26	0.06	0.06
	assign	(segid 3A4 and resid 352 and name CA)	(segid 3A4 and resid 353 and name N)	2.45	0.02	0.01
	assign	(segid 3A4 and resid 352 and name CA)	(segid 3A4 and resid 353 and name O)	4.80	0.16	0.15
30	assign	(segid 3A4 and resid 352 and name CA)	(segid 3A4 and resid 353 and name OD1)	6.73	0.09	0.08
	assign	(segid 3A4 and resid 352 and name CA)	(segid 3A4 and resid 354 and name C)	7.24	0.05	0.06
	assign	(segid 3A4 and resid 352 and name CA)	(segid 3A4 and resid 354 and name CA)	6.16	0.08	0.08
	assign	(segid 3A4 and resid 352 and name CA)	(segid 3A4 and resid 354 and name CB)	7.00	0.12	0.13
	assign	(segid 3A4 and resid 352 and name CA)	(segid 3A4 and resid 354 and name N)	5.13	0.06	0.06
35	assign	(segid 3A4 and resid 352 and name CA)	(segid 3A4 and resid 355 and name CA)	8.80	0.07	0.08
	assign	(segid 3A4 and resid 352 and name CA)	(segid 3A4 and resid 355 and name CB)	9.46	0.19	0.19
	assign	(segid 3A4 and resid 352 and name CA)	(segid 3A4 and resid 355 and name N)	7.60	0.04	0.05
	assign	(segid 3A4 and resid 352 and name CA)	(segid 3A4 and resid 356 and name C)	7.66	0.17	0.16
	assign	(segid 3A4 and resid 352 and name CA)	(segid 3A4 and resid 356 and name CA)	7.91	0.19	0.19
40	assign	(segid 3A4 and resid 352 and name CA)	(segid 3A4 and resid 356 and name CB)	7.36	0.29	0.30
	assign	(segid 3A4 and resid 352 and name CA)	(segid 3A4 and resid 356 and name N)	7.67	0.14	0.13
	assign	(segid 3A4 and resid 352 and name CA)	(segid 3A4 and resid 357 and name C)	7.00	0.29	0.29
	assign	(segid 3A4 and resid 352 and name CA)	(segid 3A4 and resid 357 and name CA)	6.70	0.18	0.17
	assign	(segid 3A4 and resid 352 and name CA)	(segid 3A4 and resid 357 and name CB)	5.64	0.20	0.20
	assign	(segid 3A4 and resid 352 and name CA)	(segid 3A4 and resid 357 and name N)	6.62	0.13	0.13
45	assign	(segid 3A4 and resid 352 and name CA)	(segid 3A4 and resid 358 and name CA)	8.75	0.16	0.16
	assign	(segid 3A4 and resid 352 and name CA)	(segid 3A4 and resid 358 and name CB)	10.18	0.16	0.15
	assign	(segid 3A4 and resid 352 and name CA)	(segid 3A4 and resid 359 and name CA)	8.51	0.28	0.28
	assign	(segid 3A4 and resid 352 and name CA)	(segid 3A4 and resid 359 and name CB)	9.83	0.25	0.24
50	assign	(segid 3A4 and resid 352 and name CA)	(segid 3A4 and resid 360 and name C)	5.25	0.19	0.19
	assign	(segid 3A4 and resid 352 and name CA)	(segid 3A4 and resid 360 and name CA)	4.97	0.22	0.22
	assign	(segid 3A4 and resid 352 and name CA)	(segid 3A4 and resid 360 and name CB)	3.81	0.26	0.27
	assign	(segid 3A4 and resid 352 and name CA)	(segid 3A4 and resid 360 and name N)	6.12	0.27	0.27
	assign	(segid 3A4 and resid 352 and name CA)	(segid 3A4 and resid 360 and name O)	5.11	0.15	0.14
55	assign	(segid 3A4 and resid 352 and name CA)	(segid 3A4 and resid 361 and name CA)	6.83	0.19	0.20
	assign	(segid 3A4 and resid 352 and name CA)	(segid 3A4 and resid 361 and name CB)	7.45	0.23	0.23
	assign	(segid 3A4 and resid 352 and name CA)	(segid 3A4 and resid 361 and name N)	6.09	0.21	0.22
	assign	(segid 3A4 and resid 352 and name CA)	(segid 3A4 and resid 362 and name CA)	9.67	0.22	0.23
	assign	(segid 3A4 and resid 352 and name CA)	(segid 3A4 and resid 362 and name CB)	10.44	0.24	0.24
60	assign	(segid 3A4 and resid 352 and name CA)	(segid 3A4 and resid 363 and name CA)	11.04	0.32	0.32
	assign	(segid 3A4 and resid 352 and name CA)	(segid 3A4 and resid 363 and name CB)	11.90	0.41	0.41
	assign	(segid 3A4 and resid 352 and name CA)	(segid 3A4 and resid 364 and name CA)	12.78	0.17	0.17
	assign	(segid 3A4 and resid 352 and name CA)	(segid 3A4 and resid 364 and name CB)	12.55	0.17	0.17
	assign	(segid 3A4 and resid 352 and name CA)	(segid 3A4 and resid 365 and name CA)	14.72	0.34	0.35
65	assign	(segid 3A4 and resid 352 and name CA)	(segid 3A4 and resid 365 and name CB)	15.99	0.29	0.30
	assign	(segid 3A4 and resid 352 and name CA)	(segid 3A4 and resid 381 and name CA)	9.04	0.55	0.55
	assign	(segid 3A4 and resid 352 and name CA)	(segid 3A4 and resid 382 and name CA)	10.41	0.55	0.56
	assign	(segid 3A4 and resid 352 and name CA)	(segid 3A4 and resid 382 and name CB)	10.25	0.65	0.64
	assign	(segid 3A4 and resid 352 and name CA)	(segid 3A4 and resid 383 and name CA)	11.13	0.59	0.59
70	assign	(segid 3A4 and resid 352 and name CA)	(segid 3A4 and resid 384 and name CA)	14.76	0.59	0.58
	assign	(segid 3A4 and resid 352 and name CA)	(segid 3A4 and resid 384 and name CB)	15.64	0.56	0.56
	assign	(segid 3A4 and resid 352 and name CA)	(segid 3A4 and resid 385 and name CA)	14.62	0.71	0.72
	assign	(segid 3A4 and resid 352 and name CA)	(segid 3A4 and resid 386 and name CA)	16.11	0.72	0.73
	assign	(segid 3A4 and resid 352 and name CA)	(segid 3A4 and resid 429 and name CA)	18.32	0.92	0.91
75	assign	(segid 3A4 and resid 352 and name CA)	(segid 3A4 and resid 433 and name CA)	15.46	0.80	0.80
	assign	(segid 3A4 and resid 352 and name CA)	(segid 3A4 and resid 434 and name CA)	17.18	0.76	0.77
	assign	(segid 3A4 and resid 352 and name CB)	(segid 3A4 and resid 352 and name CG)	1.52	0.01	0.01
	assign	(segid 3A4 and resid 352 and name CB)	(segid 3A4 and resid 353 and name C)	5.56	0.07	0.07
	assign	(segid 3A4 and resid 352 and name CB)	(segid 3A4 and resid 353 and name CA)	4.86	0.03	0.03
80	assign	(segid 3A4 and resid 352 and name CB)	(segid 3A4 and resid 353 and name CB)	5.96	0.10	0.09
	assign	(segid 3A4 and resid 352 and name CB)	(segid 3A4 and resid 353 and name CG)	7.25	0.10	0.10
	assign	(segid 3A4 and resid 352 and name CB)	(segid 3A4 and resid 353 and name N)	3.62	0.04	0.05
	assign	(segid 3A4 and resid 352 and name CB)	(segid 3A4 and resid 353 and name O)	6.10	0.18	0.17
	assign	(segid 3A4 and resid 352 and name CB)	(segid 3A4 and resid 353 and name OD1)	7.68	0.14	0.13

	assign (segid 3A4 and resid 352 and name CB) (segid 3A4 and resid 354 and name CA)	7.05	0.15	0.16
	assign (segid 3A4 and resid 352 and name CB) (segid 3A4 and resid 354 and name CB)	7.65	0.24	0.23
	assign (segid 3A4 and resid 352 and name CB) (segid 3A4 and resid 354 and name N)	6.03	0.11	0.10
5	assign (segid 3A4 and resid 352 and name CB) (segid 3A4 and resid 355 and name CA)	9.96	0.07	0.07
	assign (segid 3A4 and resid 352 and name CB) (segid 3A4 and resid 355 and name CB)	10.57	0.19	0.18
	assign (segid 3A4 and resid 352 and name CB) (segid 3A4 and resid 356 and name CA)	9.36	0.18	0.18
	assign (segid 3A4 and resid 352 and name CB) (segid 3A4 and resid 356 and name CB)	8.84	0.31	0.31
	assign (segid 3A4 and resid 352 and name CB) (segid 3A4 and resid 357 and name CA)	8.05	0.20	0.20
10	assign (segid 3A4 and resid 352 and name CB) (segid 3A4 and resid 357 and name CB)	6.98	0.23	0.23
	assign (segid 3A4 and resid 352 and name CB) (segid 3A4 and resid 358 and name CA)	9.65	0.25	0.26
	assign (segid 3A4 and resid 352 and name CB) (segid 3A4 and resid 358 and name CB)	11.09	0.30	0.29
	assign (segid 3A4 and resid 352 and name CB) (segid 3A4 and resid 359 and name CA)	8.94	0.36	0.37
	assign (segid 3A4 and resid 352 and name CB) (segid 3A4 and resid 359 and name CB)	10.23	0.38	0.38
15	assign (segid 3A4 and resid 352 and name CB) (segid 3A4 and resid 360 and name C)	5.33	0.31	0.30
	assign (segid 3A4 and resid 352 and name CB) (segid 3A4 and resid 360 and name CA)	5.41	0.31	0.30
	assign (segid 3A4 and resid 352 and name CB) (segid 3A4 and resid 360 and name CB)	4.34	0.30	0.31
	assign (segid 3A4 and resid 352 and name CB) (segid 3A4 and resid 360 and name N)	6.56	0.35	0.35
	assign (segid 3A4 and resid 352 and name CB) (segid 3A4 and resid 360 and name O)	5.15	0.29	0.28
20	assign (segid 3A4 and resid 352 and name CB) (segid 3A4 and resid 361 and name CA)	6.39	0.29	0.30
	assign (segid 3A4 and resid 352 and name CB) (segid 3A4 and resid 361 and name CB)	6.80	0.28	0.29
	assign (segid 3A4 and resid 352 and name CB) (segid 3A4 and resid 361 and name N)	5.92	0.32	0.32
	assign (segid 3A4 and resid 352 and name CB) (segid 3A4 and resid 362 and name CA)	9.61	0.32	0.31
	assign (segid 3A4 and resid 352 and name CB) (segid 3A4 and resid 362 and name CB)	10.51	0.32	0.31
25	assign (segid 3A4 and resid 352 and name CB) (segid 3A4 and resid 363 and name CA)	11.08	0.38	0.39
	assign (segid 3A4 and resid 352 and name CB) (segid 3A4 and resid 363 and name CB)	11.81	0.44	0.45
	assign (segid 3A4 and resid 352 and name CB) (segid 3A4 and resid 364 and name CA)	13.22	0.27	0.27
	assign (segid 3A4 and resid 352 and name CB) (segid 3A4 and resid 364 and name CB)	13.07	0.30	0.29
	assign (segid 3A4 and resid 352 and name CB) (segid 3A4 and resid 365 and name CA)	15.32	0.35	0.34
30	assign (segid 3A4 and resid 352 and name CB) (segid 3A4 and resid 365 and name CB)	16.52	0.26	0.25
	assign (segid 3A4 and resid 352 and name CB) (segid 3A4 and resid 381 and name CA)	10.12	0.62	0.63
	assign (segid 3A4 and resid 352 and name CB) (segid 3A4 and resid 382 and name CA)	11.18	0.58	0.57
	assign (segid 3A4 and resid 352 and name CB) (segid 3A4 and resid 382 and name CB)	10.99	0.63	0.63
	assign (segid 3A4 and resid 352 and name CB) (segid 3A4 and resid 383 and name CA)	11.52	0.65	0.65
35	assign (segid 3A4 and resid 352 and name CB) (segid 3A4 and resid 384 and name CA)	15.20	0.64	0.64
	assign (segid 3A4 and resid 352 and name CB) (segid 3A4 and resid 384 and name CB)	16.17	0.62	0.61
	assign (segid 3A4 and resid 352 and name CB) (segid 3A4 and resid 385 and name CA)	15.11	0.73	0.74
	assign (segid 3A4 and resid 352 and name CB) (segid 3A4 and resid 386 and name CA)	16.86	0.74	0.73
	assign (segid 3A4 and resid 352 and name CB) (segid 3A4 and resid 426 and name CA)	17.22	1.54	1.54
40	assign (segid 3A4 and resid 352 and name CB) (segid 3A4 and resid 427 and name CA)	17.27	1.18	1.18
	assign (segid 3A4 and resid 352 and name CB) (segid 3A4 and resid 428 and name CA)	17.78	1.25	1.24
	assign (segid 3A4 and resid 352 and name CB) (segid 3A4 and resid 429 and name CA)	17.16	1.02	1.03
	assign (segid 3A4 and resid 352 and name CB) (segid 3A4 and resid 433 and name CA)	14.53	0.87	0.86
	assign (segid 3A4 and resid 352 and name CB) (segid 3A4 and resid 434 and name CA)	16.27	0.81	0.82
45	assign (segid 3A4 and resid 352 and name CB) (segid 3A4 and resid 435 and name CA)	17.99	0.86	0.87
	assign (segid 3A4 and resid 352 and name CG) (segid 3A4 and resid 353 and name C)	6.89	0.10	0.11
	assign (segid 3A4 and resid 352 and name CG) (segid 3A4 and resid 353 and name CA)	6.25	0.01	0.01
	assign (segid 3A4 and resid 352 and name CG) (segid 3A4 and resid 353 and name CB)	7.26	0.09	0.09
	assign (segid 3A4 and resid 352 and name CG) (segid 3A4 and resid 353 and name N)	4.93	0.02	0.02
50	assign (segid 3A4 and resid 352 and name CG) (segid 3A4 and resid 353 and name O)	7.29	0.23	0.22
	assign (segid 3A4 and resid 352 and name CG) (segid 3A4 and resid 354 and name N)	7.40	0.15	0.16
	assign (segid 3A4 and resid 352 and name CG) (segid 3A4 and resid 360 and name C)	5.19	0.42	0.41
	assign (segid 3A4 and resid 352 and name CG) (segid 3A4 and resid 360 and name CA)	5.62	0.41	0.40
	assign (segid 3A4 and resid 352 and name CG) (segid 3A4 and resid 360 and name CB)	4.90	0.34	0.35
55	assign (segid 3A4 and resid 352 and name CG) (segid 3A4 and resid 360 and name N)	6.91	0.41	0.41
	assign (segid 3A4 and resid 352 and name CG) (segid 3A4 and resid 360 and name O)	4.71	0.43	0.44
	assign (segid 3A4 and resid 352 and name CG) (segid 3A4 and resid 361 and name CA)	5.99	0.37	0.36
	assign (segid 3A4 and resid 352 and name CG) (segid 3A4 and resid 361 and name CB)	6.50	0.33	0.32
	assign (segid 3A4 and resid 352 and name CG) (segid 3A4 and resid 361 and name N)	5.79	0.39	0.38
60	assign (segid 3A4 and resid 352 and name N) (segid 3A4 and resid 352 and name C)	2.47	0.03	0.02
	assign (segid 3A4 and resid 352 and name N) (segid 3A4 and resid 352 and name CA)	1.45	0.00	0.01
	assign (segid 3A4 and resid 352 and name N) (segid 3A4 and resid 352 and name CB)	2.46	0.02	0.02
	assign (segid 3A4 and resid 352 and name N) (segid 3A4 and resid 352 and name CG)	3.07	0.07	0.07
	assign (segid 3A4 and resid 352 and name N) (segid 3A4 and resid 352 and name O)	3.60	0.02	0.02
65	assign (segid 3A4 and resid 352 and name N) (segid 3A4 and resid 353 and name C)	4.98	0.08	0.07
	assign (segid 3A4 and resid 352 and name N) (segid 3A4 and resid 353 and name CA)	4.14	0.04	0.05
	assign (segid 3A4 and resid 352 and name N) (segid 3A4 and resid 353 and name CB)	4.76	0.07	0.08
	assign (segid 3A4 and resid 352 and name N) (segid 3A4 and resid 353 and name CG)	6.25	0.08	0.08
	assign (segid 3A4 and resid 352 and name N) (segid 3A4 and resid 353 and name N)	2.70	0.04	0.05
70	assign (segid 3A4 and resid 352 and name N) (segid 3A4 and resid 353 and name O)	5.17	0.13	0.14
	assign (segid 3A4 and resid 352 and name N) (segid 3A4 and resid 353 and name OD1)	6.95	0.09	0.09
	assign (segid 3A4 and resid 352 and name N) (segid 3A4 and resid 354 and name CA)	7.02	0.06	0.06
	assign (segid 3A4 and resid 352 and name N) (segid 3A4 and resid 354 and name N)	5.91	0.07	0.07
	assign (segid 3A4 and resid 352 and name N) (segid 3A4 and resid 356 and name CB)	7.05	0.42	0.42
75	assign (segid 3A4 and resid 352 and name N) (segid 3A4 and resid 357 and name CA)	7.00	0.19	0.20
	assign (segid 3A4 and resid 352 and name N) (segid 3A4 and resid 357 and name CB)	5.88	0.17	0.17
	assign (segid 3A4 and resid 352 and name N) (segid 3A4 and resid 357 and name N)	6.83	0.24	0.24
	assign (segid 3A4 and resid 352 and name N) (segid 3A4 and resid 360 and name C)	6.32	0.15	0.14
	assign (segid 3A4 and resid 352 and name N) (segid 3A4 and resid 360 and name CA)	6.05	0.19	0.18
80	assign (segid 3A4 and resid 352 and name N) (segid 3A4 and resid 360 and name CB)	5.02	0.26	0.26
	assign (segid 3A4 and resid 352 and name N) (segid 3A4 and resid 360 and name N)	7.27	0.24	0.23
	assign (segid 3A4 and resid 352 and name N) (segid 3A4 and resid 360 and name O)	5.97	0.09	0.10
	assign (segid 3A4 and resid 352 and name N) (segid 3A4 and resid 361 and name N)	7.27	0.16	0.17
	assign (segid 3A4 and resid 352 and name O) (segid 3A4 and resid 352 and name CB)	2.86	0.07	0.07

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	assign (segid 3A4 and resid 353 and name CA) (segid 3A4 and resid 357 and name C)	6.38	0.25	0.25
	assign (segid 3A4 and resid 353 and name CA) (segid 3A4 and resid 357 and name CA)	6.08	0.11	0.11
	assign (segid 3A4 and resid 353 and name CA) (segid 3A4 and resid 357 and name CB)	5.83	0.16	0.17
	assign (segid 3A4 and resid 353 and name CA) (segid 3A4 and resid 357 and name N)	5.24	0.09	0.08
5	assign (segid 3A4 and resid 353 and name CA) (segid 3A4 and resid 358 and name CA)	8.19	0.24	0.24
	assign (segid 3A4 and resid 353 and name CA) (segid 3A4 and resid 358 and name CB)	9.53	0.19	0.20
	assign (segid 3A4 and resid 353 and name CA) (segid 3A4 and resid 359 and name CA)	9.23	0.46	0.45
	assign (segid 3A4 and resid 353 and name CA) (segid 3A4 and resid 359 and name CB)	10.67	0.37	0.37
	assign (segid 3A4 and resid 353 and name CA) (segid 3A4 and resid 360 and name CA)	6.78	0.32	0.33
10	assign (segid 3A4 and resid 353 and name CA) (segid 3A4 and resid 360 and name CB)	5.35	0.35	0.34
	assign (segid 3A4 and resid 353 and name CA) (segid 3A4 and resid 361 and name CA)	9.54	0.31	0.32
	assign (segid 3A4 and resid 353 and name CA) (segid 3A4 and resid 361 and name CB)	9.97	0.35	0.35
	assign (segid 3A4 and resid 353 and name CA) (segid 3A4 and resid 362 and name CA)	12.19	0.36	0.36
	assign (segid 3A4 and resid 353 and name CA) (segid 3A4 and resid 362 and name CB)	12.58	0.41	0.40
15	assign (segid 3A4 and resid 353 and name CA) (segid 3A4 and resid 363 and name CA)	13.97	0.38	0.39
	assign (segid 3A4 and resid 353 and name CA) (segid 3A4 and resid 363 and name CB)	15.04	0.45	0.45
	assign (segid 3A4 and resid 353 and name CA) (segid 3A4 and resid 364 and name CA)	15.06	0.31	0.30
	assign (segid 3A4 and resid 353 and name CA) (segid 3A4 and resid 364 and name CB)	14.53	0.30	0.30
	assign (segid 3A4 and resid 353 and name CA) (segid 3A4 and resid 365 and name CA)	16.96	0.57	0.58
20	assign (segid 3A4 and resid 353 and name CA) (segid 3A4 and resid 365 and name CB)	18.36	0.55	0.55
	assign (segid 3A4 and resid 353 and name CA) (segid 3A4 and resid 381 and name CA)	9.87	0.33	0.33
	assign (segid 3A4 and resid 353 and name CA) (segid 3A4 and resid 382 and name CA)	11.28	0.49	0.49
	assign (segid 3A4 and resid 353 and name CA) (segid 3A4 and resid 382 and name CB)	10.76	0.60	0.61
	assign (segid 3A4 and resid 353 and name CA) (segid 3A4 and resid 383 and name CA)	13.09	0.49	0.50
25	assign (segid 3A4 and resid 353 and name CA) (segid 3A4 and resid 384 and name CA)	16.34	0.50	0.50
	assign (segid 3A4 and resid 353 and name CA) (segid 3A4 and resid 384 and name CB)	17.19	0.46	0.47
	assign (segid 3A4 and resid 353 and name CA) (segid 3A4 and resid 385 and name CA)	15.48	0.66	0.66
	assign (segid 3A4 and resid 353 and name CA) (segid 3A4 and resid 386 and name CA)	16.14	0.71	0.70
	assign (segid 3A4 and resid 353 and name CA) (segid 3A4 and resid 433 and name CA)	18.71	0.72	0.71
30	assign (segid 3A4 and resid 353 and name CB) (segid 3A4 and resid 353 and name CG)	1.52	0.01	0.01
	assign (segid 3A4 and resid 353 and name CB) (segid 3A4 and resid 353 and name OD1)	2.43	0.04	0.03
	assign (segid 3A4 and resid 353 and name CB) (segid 3A4 and resid 354 and name C)	5.02	0.06	0.07
	assign (segid 3A4 and resid 353 and name CB) (segid 3A4 and resid 354 and name CA)	4.76	0.04	0.04
	assign (segid 3A4 and resid 353 and name CB) (segid 3A4 and resid 354 and name CB)	5.84	0.08	0.08
35	assign (segid 3A4 and resid 353 and name CB) (segid 3A4 and resid 354 and name N)	3.50	0.05	0.05
	assign (segid 3A4 and resid 353 and name CB) (segid 3A4 and resid 354 and name O)	6.05	0.12	0.12
	assign (segid 3A4 and resid 353 and name CB) (segid 3A4 and resid 355 and name C)	5.37	0.10	0.11
	assign (segid 3A4 and resid 353 and name CB) (segid 3A4 and resid 355 and name CA)	5.31	0.15	0.15
	assign (segid 3A4 and resid 353 and name CB) (segid 3A4 and resid 355 and name CB)	5.36	0.26	0.27
40	assign (segid 3A4 and resid 353 and name CB) (segid 3A4 and resid 355 and name N)	4.49	0.09	0.09
	assign (segid 3A4 and resid 353 and name CB) (segid 3A4 and resid 355 and name O)	6.47	0.12	0.12
	assign (segid 3A4 and resid 353 and name CB) (segid 3A4 and resid 356 and name C)	5.85	0.13	0.12
	assign (segid 3A4 and resid 353 and name CB) (segid 3A4 and resid 356 and name CA)	5.13	0.13	0.13
	assign (segid 3A4 and resid 353 and name CB) (segid 3A4 and resid 356 and name CB)	4.46	0.19	0.19
45	assign (segid 3A4 and resid 353 and name CB) (segid 3A4 and resid 356 and name N)	4.51	0.07	0.08
	assign (segid 3A4 and resid 353 and name CB) (segid 3A4 and resid 356 and name O)	7.01	0.13	0.13
	assign (segid 3A4 and resid 353 and name CB) (segid 3A4 and resid 357 and name C)	7.07	0.20	0.20
	assign (segid 3A4 and resid 353 and name CB) (segid 3A4 and resid 357 and name CA)	6.52	0.16	0.15
	assign (segid 3A4 and resid 353 and name CB) (segid 3A4 and resid 357 and name CB)	6.39	0.22	0.21
50	assign (segid 3A4 and resid 353 and name CB) (segid 3A4 and resid 357 and name N)	5.45	0.14	0.13
	assign (segid 3A4 and resid 353 and name CB) (segid 3A4 and resid 358 and name CA)	9.10	0.36	0.36
	assign (segid 3A4 and resid 353 and name CB) (segid 3A4 and resid 358 and name CB)	10.36	0.31	0.32
	assign (segid 3A4 and resid 353 and name CB) (segid 3A4 and resid 359 and name CA)	10.49	0.44	0.45
	assign (segid 3A4 and resid 353 and name CB) (segid 3A4 and resid 359 and name CB)	11.91	0.34	0.34
55	assign (segid 3A4 and resid 353 and name CB) (segid 3A4 and resid 360 and name CA)	8.08	0.32	0.32
	assign (segid 3A4 and resid 353 and name CB) (segid 3A4 and resid 360 and name CB)	6.71	0.33	0.34
	assign (segid 3A4 and resid 353 and name CB) (segid 3A4 and resid 361 and name CA)	10.95	0.30	0.30
	assign (segid 3A4 and resid 353 and name CB) (segid 3A4 and resid 361 and name CB)	11.44	0.33	0.33
	assign (segid 3A4 and resid 353 and name CB) (segid 3A4 and resid 362 and name CA)	13.47	0.35	0.36
60	assign (segid 3A4 and resid 353 and name CB) (segid 3A4 and resid 362 and name CB)	13.85	0.39	0.40
	assign (segid 3A4 and resid 353 and name CB) (segid 3A4 and resid 363 and name CA)	15.03	0.37	0.38
	assign (segid 3A4 and resid 353 and name CB) (segid 3A4 and resid 363 and name CB)	16.10	0.43	0.43
	assign (segid 3A4 and resid 353 and name CB) (segid 3A4 and resid 364 and name CA)	15.95	0.37	0.37
	assign (segid 3A4 and resid 353 and name CB) (segid 3A4 and resid 364 and name CB)	15.44	0.36	0.35
65	assign (segid 3A4 and resid 353 and name CB) (segid 3A4 and resid 365 and name CA)	17.59	0.69	0.70
	assign (segid 3A4 and resid 353 and name CB) (segid 3A4 and resid 365 and name CB)	18.99	0.67	0.67
	assign (segid 3A4 and resid 353 and name CB) (segid 3A4 and resid 381 and name CA)	9.32	0.27	0.28
	assign (segid 3A4 and resid 353 and name CB) (segid 3A4 and resid 382 and name CA)	10.55	0.47	0.47
	assign (segid 3A4 and resid 353 and name CB) (segid 3A4 and resid 382 and name CB)	9.91	0.58	0.59
70	assign (segid 3A4 and resid 353 and name CB) (segid 3A4 and resid 383 and name CA)	12.74	0.47	0.48
	assign (segid 3A4 and resid 353 and name CB) (segid 3A4 and resid 384 and name CA)	15.78	0.49	0.48
	assign (segid 3A4 and resid 353 and name CB) (segid 3A4 and resid 384 and name CB)	16.62	0.45	0.44
	assign (segid 3A4 and resid 353 and name CB) (segid 3A4 and resid 385 and name CA)	14.66	0.66	0.66
	assign (segid 3A4 and resid 353 and name CB) (segid 3A4 and resid 386 and name CA)	15.04	0.70	0.71
75	assign (segid 3A4 and resid 353 and name CB) (segid 3A4 and resid 387 and name CA)	17.98	0.72	0.72
	assign (segid 3A4 and resid 353 and name CB) (segid 3A4 and resid 390 and name CB)	18.78	0.53	0.53
	assign (segid 3A4 and resid 353 and name CG) (segid 3A4 and resid 353 and name OD1)	1.26	0.03	0.03
	assign (segid 3A4 and resid 353 and name CG) (segid 3A4 and resid 354 and name C)	4.83	0.05	0.06
80	assign (segid 3A4 and resid 353 and name CG) (segid 3A4 and resid 354 and name CA)	4.84	0.11	0.12
	assign (segid 3A4 and resid 353 and name CG) (segid 3A4 and resid 354 and name CB)	5.74	0.16	0.16
	assign (segid 3A4 and resid 353 and name CG) (segid 3A4 and resid 354 and name N)	3.73	0.13	0.14
	assign (segid 3A4 and resid 353 and name CG) (segid 3A4 and resid 354 and name O)	5.92	0.02	0.02
	assign (segid 3A4 and resid 353 and name CG) (segid 3A4 and resid 355 and name C)	4.93	0.09	0.10

	assign (segid 3A4 and resid 353 and name CG)	(segid 3A4 and resid 355 and name CA)	4.61	0.13	0.13
	assign (segid 3A4 and resid 353 and name CG)	(segid 3A4 and resid 355 and name CB)	4.30	0.25	0.25
	assign (segid 3A4 and resid 353 and name CG)	(segid 3A4 and resid 355 and name N)	3.97	0.09	0.09
	assign (segid 3A4 and resid 353 and name CG)	(segid 3A4 and resid 355 and name O)	6.00	0.11	0.12
5	assign (segid 3A4 and resid 353 and name CG)	(segid 3A4 and resid 356 and name C)	6.26	0.22	0.21
	assign (segid 3A4 and resid 353 and name CG)	(segid 3A4 and resid 356 and name CA)	5.27	0.21	0.21
	assign (segid 3A4 and resid 353 and name CG)	(segid 3A4 and resid 356 and name CB)	4.79	0.25	0.26
	assign (segid 3A4 and resid 353 and name CG)	(segid 3A4 and resid 356 and name N)	4.40	0.16	0.16
	assign (segid 3A4 and resid 353 and name CG)	(segid 3A4 and resid 356 and name O)	7.43	0.22	0.21
10	assign (segid 3A4 and resid 353 and name CG)	(segid 3A4 and resid 357 and name CA)	7.27	0.22	0.21
	assign (segid 3A4 and resid 353 and name CG)	(segid 3A4 and resid 357 and name CB)	7.41	0.25	0.24
	assign (segid 3A4 and resid 353 and name CG)	(segid 3A4 and resid 357 and name N)	6.04	0.21	0.21
	assign (segid 3A4 and resid 353 and name CG)	(segid 3A4 and resid 353 and name C)	2.43	0.03	0.03
	assign (segid 3A4 and resid 353 and name N)	(segid 3A4 and resid 353 and name CA)	1.46	0.00	0.00
15	assign (segid 3A4 and resid 353 and name N)	(segid 3A4 and resid 353 and name CB)	2.45	0.02	0.02
	assign (segid 3A4 and resid 353 and name N)	(segid 3A4 and resid 353 and name CG)	3.83	0.04	0.04
	assign (segid 3A4 and resid 353 and name N)	(segid 3A4 and resid 353 and name O)	2.96	0.06	0.07
	assign (segid 3A4 and resid 353 and name N)	(segid 3A4 and resid 353 and name OD1)	4.34	0.07	0.08
20	assign (segid 3A4 and resid 353 and name N)	(segid 3A4 and resid 354 and name C)	5.50	0.08	0.08
	assign (segid 3A4 and resid 353 and name N)	(segid 3A4 and resid 354 and name CA)	4.67	0.05	0.04
	assign (segid 3A4 and resid 353 and name N)	(segid 3A4 and resid 354 and name CB)	5.70	0.06	0.06
	assign (segid 3A4 and resid 353 and name N)	(segid 3A4 and resid 354 and name N)	3.40	0.04	0.04
	assign (segid 3A4 and resid 353 and name N)	(segid 3A4 and resid 354 and name O)	6.41	0.17	0.16
	assign (segid 3A4 and resid 353 and name N)	(segid 3A4 and resid 355 and name C)	6.70	0.10	0.10
25	assign (segid 3A4 and resid 353 and name N)	(segid 3A4 and resid 355 and name CA)	6.68	0.11	0.12
	assign (segid 3A4 and resid 353 and name N)	(segid 3A4 and resid 355 and name CB)	7.16	0.21	0.22
	assign (segid 3A4 and resid 353 and name N)	(segid 3A4 and resid 355 and name N)	5.55	0.07	0.08
	assign (segid 3A4 and resid 353 and name N)	(segid 3A4 and resid 355 and name O)	7.83	0.08	0.07
	assign (segid 3A4 and resid 353 and name N)	(segid 3A4 and resid 356 and name C)	6.26	0.10	0.10
30	assign (segid 3A4 and resid 353 and name N)	(segid 3A4 and resid 356 and name CA)	6.12	0.13	0.14
	assign (segid 3A4 and resid 353 and name N)	(segid 3A4 and resid 356 and name CB)	5.57	0.22	0.22
	assign (segid 3A4 and resid 353 and name N)	(segid 3A4 and resid 356 and name N)	5.68	0.10	0.11
	assign (segid 3A4 and resid 353 and name N)	(segid 3A4 and resid 356 and name O)	7.36	0.12	0.12
	assign (segid 3A4 and resid 353 and name N)	(segid 3A4 and resid 357 and name C)	6.40	0.24	0.25
35	assign (segid 3A4 and resid 353 and name N)	(segid 3A4 and resid 357 and name CA)	6.00	0.14	0.14
	assign (segid 3A4 and resid 353 and name N)	(segid 3A4 and resid 357 and name CB)	5.40	0.20	0.19
	assign (segid 3A4 and resid 353 and name N)	(segid 3A4 and resid 357 and name N)	5.42	0.11	0.10
	assign (segid 3A4 and resid 353 and name N)	(segid 3A4 and resid 357 and name O)	6.03	0.72	0.72
	assign (segid 3A4 and resid 353 and name N)	(segid 3A4 and resid 360 and name C)	6.83	0.23	0.24
40	assign (segid 3A4 and resid 353 and name N)	(segid 3A4 and resid 360 and name CA)	6.07	0.27	0.27
	assign (segid 3A4 and resid 353 and name N)	(segid 3A4 and resid 360 and name CB)	4.68	0.31	0.31
	assign (segid 3A4 and resid 353 and name N)	(segid 3A4 and resid 360 and name N)	6.87	0.35	0.34
	assign (segid 3A4 and resid 353 and name N)	(segid 3A4 and resid 360 and name O)	6.96	0.17	0.17
	assign (segid 3A4 and resid 353 and name O)	(segid 3A4 and resid 353 and name CB)	2.95	0.06	0.07
45	assign (segid 3A4 and resid 353 and name O)	(segid 3A4 and resid 353 and name CG)	3.65	0.08	0.07
	assign (segid 3A4 and resid 353 and name O)	(segid 3A4 and resid 353 and name OD1)	3.58	0.16	0.16
	assign (segid 3A4 and resid 353 and name O)	(segid 3A4 and resid 354 and name C)	3.00	0.14	0.13
	assign (segid 3A4 and resid 353 and name O)	(segid 3A4 and resid 354 and name CA)	2.79	0.04	0.03
	assign (segid 3A4 and resid 353 and name O)	(segid 3A4 and resid 354 and name CB)	4.24	0.04	0.04
50	assign (segid 3A4 and resid 353 and name O)	(segid 3A4 and resid 354 and name N)	2.25	0.01	0.00
	assign (segid 3A4 and resid 353 and name O)	(segid 3A4 and resid 354 and name O)	3.70	0.21	0.21
	assign (segid 3A4 and resid 353 and name O)	(segid 3A4 and resid 355 and name C)	3.97	0.18	0.19
	assign (segid 3A4 and resid 353 and name O)	(segid 3A4 and resid 355 and name CA)	4.15	0.19	0.19
	assign (segid 3A4 and resid 353 and name O)	(segid 3A4 and resid 355 and name CB)	5.03	0.25	0.25
55	assign (segid 3A4 and resid 353 and name O)	(segid 3A4 and resid 355 and name N)	3.17	0.13	0.13
	assign (segid 3A4 and resid 353 and name O)	(segid 3A4 and resid 355 and name O)	5.08	0.13	0.13
	assign (segid 3A4 and resid 353 and name O)	(segid 3A4 and resid 356 and name C)	3.74	0.11	0.10
	assign (segid 3A4 and resid 353 and name O)	(segid 3A4 and resid 356 and name CA)	3.64	0.18	0.19
	assign (segid 3A4 and resid 353 and name O)	(segid 3A4 and resid 356 and name CB)	3.74	0.19	0.18
60	assign (segid 3A4 and resid 353 and name O)	(segid 3A4 and resid 356 and name N)	2.99	0.23	0.24
	assign (segid 3A4 and resid 353 and name O)	(segid 3A4 and resid 356 and name O)	4.93	0.09	0.08
	assign (segid 3A4 and resid 353 and name O)	(segid 3A4 and resid 357 and name C)	4.19	0.24	0.24
	assign (segid 3A4 and resid 353 and name O)	(segid 3A4 and resid 357 and name CA)	3.86	0.10	0.10
	assign (segid 3A4 and resid 353 and name O)	(segid 3A4 and resid 357 and name CB)	4.00	0.15	0.16
65	assign (segid 3A4 and resid 353 and name O)	(segid 3A4 and resid 357 and name N)	2.93	0.06	0.06
	assign (segid 3A4 and resid 353 and name O)	(segid 3A4 and resid 357 and name O)	4.05	0.69	0.69
	assign (segid 3A4 and resid 353 and name O)	(segid 3A4 and resid 358 and name C)	6.70	0.56	0.56
	assign (segid 3A4 and resid 353 and name O)	(segid 3A4 and resid 358 and name CA)	6.24	0.43	0.43
	assign (segid 3A4 and resid 353 and name O)	(segid 3A4 and resid 358 and name N)	5.48	0.54	0.55
70	assign (segid 3A4 and resid 353 and name O)	(segid 3A4 and resid 360 and name C)	7.25	0.42	0.42
	assign (segid 3A4 and resid 353 and name O)	(segid 3A4 and resid 360 and name CA)	6.00	0.45	0.45
	assign (segid 3A4 and resid 353 and name O)	(segid 3A4 and resid 360 and name CB)	4.84	0.40	0.41
	assign (segid 3A4 and resid 353 and name O)	(segid 3A4 and resid 360 and name N)	6.31	0.51	0.51
	assign (segid 3A4 and resid 353 and name OD1)	(segid 3A4 and resid 354 and name C)	3.99	0.11	0.11
75	assign (segid 3A4 and resid 353 and name OD1)	(segid 3A4 and resid 354 and name CA)	4.09	0.13	0.14
	assign (segid 3A4 and resid 353 and name OD1)	(segid 3A4 and resid 354 and name CB)	4.85	0.22	0.21
	assign (segid 3A4 and resid 353 and name OD1)	(segid 3A4 and resid 354 and name N)	3.19	0.14	0.13
	assign (segid 3A4 and resid 353 and name OD1)	(segid 3A4 and resid 354 and name O)	5.11	0.10	0.11
80	assign (segid 3A4 and resid 353 and name OD1)	(segid 3A4 and resid 355 and name C)	4.39	0.26	0.25
	assign (segid 3A4 and resid 353 and name OD1)	(segid 3A4 and resid 355 and name CA)	3.76	0.13	0.13
	assign (segid 3A4 and resid 353 and name OD1)	(segid 3A4 and resid 355 and name CB)	3.49	0.16	0.15
	assign (segid 3A4 and resid 353 and name OD1)	(segid 3A4 and resid 355 and name N)	3.04	0.12	0.12
	assign (segid 3A4 and resid 353 and name OD1)	(segid 3A4 and resid 355 and name O)	5.50	0.23	0.22

	assign (segid 3A4 and resid 353 and name OD1)	(segid 3A4 and resid 356 and name C)	6.18	0.45	0.45
	assign (segid 3A4 and resid 353 and name OD1)	(segid 3A4 and resid 356 and name CA)	5.22	0.47	0.47
	assign (segid 3A4 and resid 353 and name OD1)	(segid 3A4 and resid 356 and name CB)	5.10	0.50	0.50
	assign (segid 3A4 and resid 353 and name OD1)	(segid 3A4 and resid 356 and name N)	4.09	0.42	0.42
5	assign (segid 3A4 and resid 353 and name OD1)	(segid 3A4 and resid 357 and name C)	7.40	0.42	0.42
	assign (segid 3A4 and resid 353 and name OD1)	(segid 3A4 and resid 357 and name CA)	7.16	0.40	0.40
	assign (segid 3A4 and resid 353 and name OD1)	(segid 3A4 and resid 357 and name N)	5.93	0.42	0.42
	assign (segid 3A4 and resid 354 and name C)	(segid 3A4 and resid 354 and name CB)	2.47	0.03	0.02
	assign (segid 3A4 and resid 354 and name C)	(segid 3A4 and resid 354 and name O)	1.23	0.01	0.01
10	assign (segid 3A4 and resid 354 and name C)	(segid 3A4 and resid 355 and name C)	3.11	0.03	0.04
	assign (segid 3A4 and resid 354 and name C)	(segid 3A4 and resid 355 and name CA)	2.43	0.01	0.02
	assign (segid 3A4 and resid 354 and name C)	(segid 3A4 and resid 355 and name CB)	3.71	0.04	0.03
	assign (segid 3A4 and resid 354 and name C)	(segid 3A4 and resid 355 and name N)	1.33	0.01	0.01
	assign (segid 3A4 and resid 354 and name C)	(segid 3A4 and resid 355 and name O)	4.14	0.07	0.06
15	assign (segid 3A4 and resid 354 and name C)	(segid 3A4 and resid 356 and name C)	4.63	0.09	0.08
	assign (segid 3A4 and resid 354 and name C)	(segid 3A4 and resid 356 and name CA)	4.45	0.10	0.10
	assign (segid 3A4 and resid 354 and name C)	(segid 3A4 and resid 356 and name CB)	5.36	0.08	0.08
	assign (segid 3A4 and resid 354 and name C)	(segid 3A4 and resid 356 and name N)	3.18	0.11	0.10
	assign (segid 3A4 and resid 354 and name C)	(segid 3A4 and resid 356 and name O)	5.66	0.11	0.11
20	assign (segid 3A4 and resid 354 and name C)	(segid 3A4 and resid 357 and name C)	4.49	0.22	0.21
	assign (segid 3A4 and resid 354 and name C)	(segid 3A4 and resid 357 and name CA)	4.92	0.10	0.10
	assign (segid 3A4 and resid 354 and name C)	(segid 3A4 and resid 357 and name CB)	5.75	0.14	0.15
	assign (segid 3A4 and resid 354 and name C)	(segid 3A4 and resid 357 and name N)	4.07	0.10	0.11
	assign (segid 3A4 and resid 354 and name C)	(segid 3A4 and resid 357 and name O)	4.33	0.62	0.63
25	assign (segid 3A4 and resid 354 and name C)	(segid 3A4 and resid 358 and name C)	6.15	0.68	0.68
	assign (segid 3A4 and resid 354 and name C)	(segid 3A4 and resid 358 and name CA)	5.33	0.49	0.49
	assign (segid 3A4 and resid 354 and name C)	(segid 3A4 and resid 358 and name CB)	6.37	0.39	0.38
	assign (segid 3A4 and resid 354 and name C)	(segid 3A4 and resid 358 and name N)	5.04	0.43	0.43
	assign (segid 3A4 and resid 354 and name C)	(segid 3A4 and resid 359 and name N)	6.52	0.55	0.55
30	assign (segid 3A4 and resid 354 and name C)	(segid 3A4 and resid 360 and name CA)	7.10	0.39	0.40
	assign (segid 3A4 and resid 354 and name C)	(segid 3A4 and resid 360 and name CB)	6.11	0.30	0.30
	assign (segid 3A4 and resid 354 and name C)	(segid 3A4 and resid 360 and name N)	6.78	0.52	0.52
	assign (segid 3A4 and resid 354 and name CA)	(segid 3A4 and resid 354 and name C)	1.51	0.01	0.01
	assign (segid 3A4 and resid 354 and name CA)	(segid 3A4 and resid 354 and name CB)	1.52	0.01	0.01
35	assign (segid 3A4 and resid 354 and name CA)	(segid 3A4 and resid 354 and name O)	2.37	0.02	0.02
	assign (segid 3A4 and resid 354 and name CA)	(segid 3A4 and resid 355 and name C)	4.46	0.03	0.03
	assign (segid 3A4 and resid 354 and name CA)	(segid 3A4 and resid 355 and name CA)	3.81	0.02	0.02
	assign (segid 3A4 and resid 354 and name CA)	(segid 3A4 and resid 355 and name CB)	4.88	0.05	0.04
	assign (segid 3A4 and resid 354 and name CA)	(segid 3A4 and resid 355 and name N)	2.45	0.03	0.02
40	assign (segid 3A4 and resid 354 and name CA)	(segid 3A4 and resid 355 and name O)	5.55	0.07	0.08
	assign (segid 3A4 and resid 354 and name CA)	(segid 3A4 and resid 356 and name C)	5.37	0.05	0.06
	assign (segid 3A4 and resid 354 and name CA)	(segid 3A4 and resid 356 and name CA)	5.37	0.08	0.07
	assign (segid 3A4 and resid 354 and name CA)	(segid 3A4 and resid 356 and name CB)	6.07	0.12	0.12
	assign (segid 3A4 and resid 354 and name CA)	(segid 3A4 and resid 356 and name N)	4.23	0.08	0.07
45	assign (segid 3A4 and resid 354 and name CA)	(segid 3A4 and resid 356 and name O)	6.46	0.06	0.05
	assign (segid 3A4 and resid 354 and name CA)	(segid 3A4 and resid 357 and name C)	4.56	0.24	0.24
	assign (segid 3A4 and resid 354 and name CA)	(segid 3A4 and resid 357 and name CA)	5.11	0.08	0.08
	assign (segid 3A4 and resid 354 and name CA)	(segid 3A4 and resid 357 and name CB)	5.60	0.14	0.13
	assign (segid 3A4 and resid 354 and name CA)	(segid 3A4 and resid 357 and name N)	4.50	0.09	0.10
50	assign (segid 3A4 and resid 354 and name CA)	(segid 3A4 and resid 357 and name O)	4.09	0.78	0.79
	assign (segid 3A4 and resid 354 and name CA)	(segid 3A4 and resid 358 and name C)	5.80	0.51	0.52
	assign (segid 3A4 and resid 354 and name CA)	(segid 3A4 and resid 358 and name CA)	5.33	0.29	0.29
	assign (segid 3A4 and resid 354 and name CA)	(segid 3A4 and resid 358 and name CB)	6.55	0.26	0.26
	assign (segid 3A4 and resid 354 and name CA)	(segid 3A4 and resid 358 and name N)	5.19	0.27	0.27
55	assign (segid 3A4 and resid 354 and name CA)	(segid 3A4 and resid 358 and name O)	6.27	1.01	1.01
	assign (segid 3A4 and resid 354 and name CA)	(segid 3A4 and resid 359 and name C)	6.82	0.51	0.52
	assign (segid 3A4 and resid 354 and name CA)	(segid 3A4 and resid 359 and name CA)	6.84	0.56	0.56
	assign (segid 3A4 and resid 354 and name CA)	(segid 3A4 and resid 359 and name CB)	8.25	0.49	0.49
	assign (segid 3A4 and resid 354 and name CA)	(segid 3A4 and resid 359 and name N)	6.03	0.46	0.46
60	assign (segid 3A4 and resid 354 and name CA)	(segid 3A4 and resid 360 and name CA)	6.07	0.39	0.38
	assign (segid 3A4 and resid 354 and name CA)	(segid 3A4 and resid 360 and name CB)	4.94	0.31	0.31
	assign (segid 3A4 and resid 354 and name CA)	(segid 3A4 and resid 360 and name N)	5.80	0.48	0.49
	assign (segid 3A4 and resid 354 and name CA)	(segid 3A4 and resid 361 and name CA)	9.15	0.43	0.44
	assign (segid 3A4 and resid 354 and name CA)	(segid 3A4 and resid 361 and name CB)	9.46	0.47	0.47
65	assign (segid 3A4 and resid 354 and name CA)	(segid 3A4 and resid 362 and name CA)	11.26	0.50	0.50
	assign (segid 3A4 and resid 354 and name CA)	(segid 3A4 and resid 362 and name CB)	11.21	0.56	0.55
	assign (segid 3A4 and resid 354 and name CA)	(segid 3A4 and resid 363 and name CA)	13.71	0.50	0.50
	assign (segid 3A4 and resid 354 and name CA)	(segid 3A4 and resid 363 and name CB)	14.98	0.53	0.53
	assign (segid 3A4 and resid 354 and name CA)	(segid 3A4 and resid 364 and name CA)	14.33	0.44	0.44
70	assign (segid 3A4 and resid 354 and name CA)	(segid 3A4 and resid 364 and name CB)	13.47	0.44	0.43
	assign (segid 3A4 and resid 354 and name CA)	(segid 3A4 and resid 365 and name CA)	16.71	0.65	0.65
	assign (segid 3A4 and resid 354 and name CA)	(segid 3A4 and resid 365 and name CB)	18.17	0.64	0.64
	assign (segid 3A4 and resid 354 and name CA)	(segid 3A4 and resid 381 and name CA)	12.33	0.42	0.41
	assign (segid 3A4 and resid 354 and name CA)	(segid 3A4 and resid 382 and name CA)	14.44	0.51	0.50
75	assign (segid 3A4 and resid 354 and name CA)	(segid 3A4 and resid 382 and name CB)	14.09	0.61	0.62
	assign (segid 3A4 and resid 354 and name CA)	(segid 3A4 and resid 383 and name CA)	16.21	0.48	0.47
	assign (segid 3A4 and resid 354 and name CB)	(segid 3A4 and resid 355 and name C)	5.53	0.05	0.05
	assign (segid 3A4 and resid 354 and name CB)	(segid 3A4 and resid 355 and name CA)	4.58	0.08	0.08
	assign (segid 3A4 and resid 354 and name CB)	(segid 3A4 and resid 355 and name CB)	5.50	0.12	0.12
80	assign (segid 3A4 and resid 354 and name CB)	(segid 3A4 and resid 355 and name N)	3.29	0.09	0.09
	assign (segid 3A4 and resid 354 and name CB)	(segid 3A4 and resid 355 and name O)	6.55	0.04	0.05
	assign (segid 3A4 and resid 354 and name CB)	(segid 3A4 and resid 356 and name C)	6.79	0.08	0.07
	assign (segid 3A4 and resid 354 and name CB)	(segid 3A4 and resid 356 and name CA)	6.76	0.09	0.09

	assign (segid 3A4 and resid 354 and name CB)	(segid 3A4 and resid 356 and name CB)	7.47	0.11	0.11
	assign (segid 3A4 and resid 354 and name CB)	(segid 3A4 and resid 356 and name N)	5.54	0.10	0.09
	assign (segid 3A4 and resid 354 and name CB)	(segid 3A4 and resid 357 and name C)	5.64	0.25	0.25
	assign (segid 3A4 and resid 354 and name CB)	(segid 3A4 and resid 357 and name CA)	6.42	0.12	0.12
5	assign (segid 3A4 and resid 354 and name CB)	(segid 3A4 and resid 357 and name CB)	6.91	0.16	0.16
	assign (segid 3A4 and resid 354 and name CB)	(segid 3A4 and resid 357 and name N)	5.93	0.12	0.12
	assign (segid 3A4 and resid 354 and name CB)	(segid 3A4 and resid 357 and name O)	5.08	0.77	0.76
	assign (segid 3A4 and resid 354 and name CB)	(segid 3A4 and resid 358 and name C)	6.12	0.56	0.56
	assign (segid 3A4 and resid 354 and name CB)	(segid 3A4 and resid 358 and name CA)	5.73	0.41	0.42
10	assign (segid 3A4 and resid 354 and name CB)	(segid 3A4 and resid 358 and name CB)	6.84	0.52	0.52
	assign (segid 3A4 and resid 354 and name CB)	(segid 3A4 and resid 358 and name N)	5.94	0.39	0.38
	assign (segid 3A4 and resid 354 and name CB)	(segid 3A4 and resid 359 and name CA)	6.89	0.58	0.58
	assign (segid 3A4 and resid 354 and name CB)	(segid 3A4 and resid 359 and name CB)	8.28	0.55	0.54
	assign (segid 3A4 and resid 354 and name CB)	(segid 3A4 and resid 359 and name N)	6.18	0.41	0.40
15	assign (segid 3A4 and resid 354 and name CB)	(segid 3A4 and resid 360 and name CA)	6.61	0.42	0.42
	assign (segid 3A4 and resid 354 and name CB)	(segid 3A4 and resid 360 and name CB)	5.52	0.38	0.37
	assign (segid 3A4 and resid 354 and name CB)	(segid 3A4 and resid 360 and name N)	6.14	0.50	0.50
	assign (segid 3A4 and resid 354 and name CB)	(segid 3A4 and resid 361 and name CA)	9.28	0.50	0.51
	assign (segid 3A4 and resid 354 and name CB)	(segid 3A4 and resid 361 and name CB)	9.36	0.54	0.55
20	assign (segid 3A4 and resid 354 and name CB)	(segid 3A4 and resid 362 and name CA)	11.52	0.56	0.56
	assign (segid 3A4 and resid 354 and name CB)	(segid 3A4 and resid 362 and name CB)	11.41	0.62	0.62
	assign (segid 3A4 and resid 354 and name CB)	(segid 3A4 and resid 363 and name CA)	14.29	0.55	0.54
	assign (segid 3A4 and resid 354 and name CB)	(segid 3A4 and resid 363 and name CB)	15.54	0.57	0.56
	assign (segid 3A4 and resid 354 and name CB)	(segid 3A4 and resid 364 and name CA)	15.04	0.49	0.50
25	assign (segid 3A4 and resid 354 and name CB)	(segid 3A4 and resid 364 and name CB)	14.13	0.49	0.50
	assign (segid 3A4 and resid 354 and name CB)	(segid 3A4 and resid 365 and name CA)	17.65	0.67	0.67
	assign (segid 3A4 and resid 354 and name CB)	(segid 3A4 and resid 365 and name CB)	19.10	0.67	0.66
	assign (segid 3A4 and resid 354 and name CB)	(segid 3A4 and resid 381 and name CA)	13.77	0.41	0.41
	assign (segid 3A4 and resid 354 and name CB)	(segid 3A4 and resid 382 and name CA)	15.79	0.51	0.50
30	assign (segid 3A4 and resid 354 and name CB)	(segid 3A4 and resid 382 and name CB)	15.40	0.62	0.61
	assign (segid 3A4 and resid 354 and name CB)	(segid 3A4 and resid 383 and name CA)	17.46	0.48	0.49
	assign (segid 3A4 and resid 354 and name N)	(segid 3A4 and resid 354 and name C)	2.50	0.03	0.03
	assign (segid 3A4 and resid 354 and name N)	(segid 3A4 and resid 354 and name CA)	1.46	0.00	0.00
	assign (segid 3A4 and resid 354 and name N)	(segid 3A4 and resid 354 and name CB)	2.43	0.04	0.04
35	assign (segid 3A4 and resid 354 and name N)	(segid 3A4 and resid 354 and name O)	3.58	0.04	0.04
	assign (segid 3A4 and resid 354 and name N)	(segid 3A4 and resid 355 and name C)	4.84	0.05	0.05
	assign (segid 3A4 and resid 354 and name N)	(segid 3A4 and resid 355 and name CA)	4.25	0.04	0.05
	assign (segid 3A4 and resid 354 and name N)	(segid 3A4 and resid 355 and name CB)	5.00	0.09	0.09
	assign (segid 3A4 and resid 354 and name N)	(segid 3A4 and resid 355 and name N)	2.83	0.04	0.04
40	assign (segid 3A4 and resid 354 and name N)	(segid 3A4 and resid 355 and name O)	6.04	0.06	0.05
	assign (segid 3A4 and resid 354 and name N)	(segid 3A4 and resid 356 and name C)	5.63	0.06	0.06
	assign (segid 3A4 and resid 354 and name N)	(segid 3A4 and resid 356 and name CA)	5.44	0.09	0.09
	assign (segid 3A4 and resid 354 and name N)	(segid 3A4 and resid 356 and name CB)	5.72	0.16	0.17
	assign (segid 3A4 and resid 354 and name N)	(segid 3A4 and resid 356 and name N)	4.35	0.07	0.08
45	assign (segid 3A4 and resid 354 and name N)	(segid 3A4 and resid 356 and name O)	6.81	0.05	0.06
	assign (segid 3A4 and resid 354 and name N)	(segid 3A4 and resid 357 and name C)	5.28	0.28	0.27
	assign (segid 3A4 and resid 354 and name N)	(segid 3A4 and resid 357 and name CA)	5.51	0.10	0.09
	assign (segid 3A4 and resid 354 and name N)	(segid 3A4 and resid 357 and name CB)	5.70	0.10	0.10
	assign (segid 3A4 and resid 354 and name N)	(segid 3A4 and resid 357 and name N)	4.77	0.07	0.08
50	assign (segid 3A4 and resid 354 and name N)	(segid 3A4 and resid 357 and name O)	4.81	0.85	0.84
	assign (segid 3A4 and resid 354 and name N)	(segid 3A4 and resid 358 and name C)	6.80	0.42	0.42
	assign (segid 3A4 and resid 354 and name N)	(segid 3A4 and resid 358 and name CA)	6.46	0.24	0.23
	assign (segid 3A4 and resid 354 and name N)	(segid 3A4 and resid 358 and name N)	6.16	0.26	0.27
	assign (segid 3A4 and resid 354 and name N)	(segid 3A4 and resid 360 and name C)	7.35	0.33	0.33
55	assign (segid 3A4 and resid 354 and name N)	(segid 3A4 and resid 360 and name CA)	6.18	0.35	0.36
	assign (segid 3A4 and resid 354 and name N)	(segid 3A4 and resid 360 and name CB)	4.83	0.31	0.32
	assign (segid 3A4 and resid 354 and name N)	(segid 3A4 and resid 360 and name N)	6.24	0.45	0.46
	assign (segid 3A4 and resid 354 and name O)	(segid 3A4 and resid 354 and name CB)	3.11	0.11	0.12
	assign (segid 3A4 and resid 354 and name O)	(segid 3A4 and resid 355 and name C)	3.14	0.11	0.10
60	assign (segid 3A4 and resid 354 and name O)	(segid 3A4 and resid 355 and name CA)	2.75	0.02	0.02
	assign (segid 3A4 and resid 354 and name O)	(segid 3A4 and resid 355 and name CB)	4.22	0.06	0.05
	assign (segid 3A4 and resid 354 and name O)	(segid 3A4 and resid 355 and name N)	2.24	0.01	0.01
	assign (segid 3A4 and resid 354 and name O)	(segid 3A4 and resid 355 and name O)	3.89	0.08	0.08
	assign (segid 3A4 and resid 354 and name O)	(segid 3A4 and resid 356 and name C)	4.36	0.28	0.28
65	assign (segid 3A4 and resid 354 and name O)	(segid 3A4 and resid 356 and name CA)	4.43	0.27	0.27
	assign (segid 3A4 and resid 354 and name O)	(segid 3A4 and resid 356 and name CB)	5.60	0.22	0.23
	assign (segid 3A4 and resid 354 and name O)	(segid 3A4 and resid 356 and name N)	3.36	0.24	0.24
	assign (segid 3A4 and resid 354 and name O)	(segid 3A4 and resid 356 and name O)	5.22	0.30	0.31
	assign (segid 3A4 and resid 354 and name O)	(segid 3A4 and resid 357 and name C)	3.94	0.20	0.20
70	assign (segid 3A4 and resid 354 and name O)	(segid 3A4 and resid 357 and name CA)	4.55	0.22	0.22
	assign (segid 3A4 and resid 354 and name O)	(segid 3A4 and resid 357 and name CB)	5.61	0.26	0.27
	assign (segid 3A4 and resid 354 and name O)	(segid 3A4 and resid 357 and name N)	3.88	0.27	0.26
	assign (segid 3A4 and resid 354 and name O)	(segid 3A4 and resid 357 and name O)	3.94	0.45	0.45
	assign (segid 3A4 and resid 354 and name O)	(segid 3A4 and resid 358 and name C)	5.50	0.76	0.77
75	assign (segid 3A4 and resid 354 and name O)	(segid 3A4 and resid 358 and name CA)	4.53	0.59	0.59
	assign (segid 3A4 and resid 354 and name O)	(segid 3A4 and resid 358 and name CB)	5.44	0.48	0.48
	assign (segid 3A4 and resid 354 and name O)	(segid 3A4 and resid 358 and name N)	4.28	0.45	0.45
	assign (segid 3A4 and resid 354 and name O)	(segid 3A4 and resid 358 and name O)	6.14	1.11	1.12
	assign (segid 3A4 and resid 354 and name O)	(segid 3A4 and resid 359 and name N)	5.94	0.59	0.59
80	assign (segid 3A4 and resid 354 and name O)	(segid 3A4 and resid 360 and name CB)	6.38	0.29	0.29
	assign (segid 3A4 and resid 354 and name O)	(segid 3A4 and resid 360 and name N)	6.66	0.52	0.52
	assign (segid 3A4 and resid 355 and name C)	(segid 3A4 and resid 355 and name CB)	2.48	0.04	0.05
	assign (segid 3A4 and resid 355 and name C)	(segid 3A4 and resid 355 and name O)	1.23	0.00	0.01

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	assign (segid 3A4 and resid 355 and name N)	(segid 3A4 and resid 357 and name O)	5.41	0.60	0.59
	assign (segid 3A4 and resid 355 and name N)	(segid 3A4 and resid 358 and name CA)	6.52	0.56	0.56
	assign (segid 3A4 and resid 355 and name N)	(segid 3A4 and resid 358 and name N)	6.10	0.53	0.52
	assign (segid 3A4 and resid 355 and name N)	(segid 3A4 and resid 360 and name CB)	7.07	0.32	0.32
5	assign (segid 3A4 and resid 355 and name O)	(segid 3A4 and resid 355 and name CB)	3.09	0.10	0.10
	assign (segid 3A4 and resid 355 and name O)	(segid 3A4 and resid 356 and name C)	3.62	0.16	0.16
	assign (segid 3A4 and resid 355 and name O)	(segid 3A4 and resid 356 and name CA)	2.74	0.05	0.06
	assign (segid 3A4 and resid 355 and name O)	(segid 3A4 and resid 356 and name CB)	4.00	0.14	0.14
	assign (segid 3A4 and resid 355 and name O)	(segid 3A4 and resid 356 and name N)	2.24	0.01	0.02
10	assign (segid 3A4 and resid 355 and name O)	(segid 3A4 and resid 357 and name C)	4.12	0.17	0.18
	assign (segid 3A4 and resid 355 and name O)	(segid 3A4 and resid 357 and name CA)	5.56	0.31	0.31
	assign (segid 3A4 and resid 355 and name O)	(segid 3A4 and resid 357 and name CB)	6.79	0.26	0.26
	assign (segid 3A4 and resid 355 and name O)	(segid 3A4 and resid 357 and name N)	4.35	0.23	0.24
15	assign (segid 3A4 and resid 355 and name O)	(segid 3A4 and resid 358 and name O)	6.40	0.23	0.23
	assign (segid 3A4 and resid 355 and name O)	(segid 3A4 and resid 358 and name N)	6.41	0.91	0.90
	assign (segid 3A4 and resid 356 and name C)	(segid 3A4 and resid 356 and name CB)	2.51	0.04	0.03
	assign (segid 3A4 and resid 356 and name C)	(segid 3A4 and resid 356 and name O)	1.23	0.00	0.00
	assign (segid 3A4 and resid 356 and name C)	(segid 3A4 and resid 357 and name C)	3.48	0.09	0.08
20	assign (segid 3A4 and resid 356 and name C)	(segid 3A4 and resid 357 and name CA)	2.44	0.02	0.01
	assign (segid 3A4 and resid 356 and name C)	(segid 3A4 and resid 357 and name CB)	3.48	0.06	0.07
	assign (segid 3A4 and resid 356 and name C)	(segid 3A4 and resid 357 and name N)	1.33	0.00	0.01
	assign (segid 3A4 and resid 356 and name C)	(segid 3A4 and resid 357 and name O)	4.24	0.14	0.13
	assign (segid 3A4 and resid 356 and name C)	(segid 3A4 and resid 358 and name N)	4.59	0.89	0.90
25	assign (segid 3A4 and resid 356 and name C)	(segid 3A4 and resid 360 and name CB)	7.03	0.24	0.24
	assign (segid 3A4 and resid 356 and name CA)	(segid 3A4 and resid 356 and name C)	1.55	0.00	0.01
	assign (segid 3A4 and resid 356 and name CA)	(segid 3A4 and resid 356 and name CB)	1.55	0.02	0.01
	assign (segid 3A4 and resid 356 and name CA)	(segid 3A4 and resid 356 and name O)	2.38	0.01	0.02
	assign (segid 3A4 and resid 356 and name CA)	(segid 3A4 and resid 357 and name C)	4.72	0.04	0.05
30	assign (segid 3A4 and resid 356 and name CA)	(segid 3A4 and resid 357 and name CA)	3.82	0.02	0.01
	assign (segid 3A4 and resid 356 and name CA)	(segid 3A4 and resid 357 and name CB)	4.71	0.04	0.04
	assign (segid 3A4 and resid 356 and name CA)	(segid 3A4 and resid 357 and name N)	2.44	0.01	0.02
	assign (segid 3A4 and resid 356 and name CA)	(segid 3A4 and resid 357 and name O)	5.32	0.24	0.23
	assign (segid 3A4 and resid 356 and name CA)	(segid 3A4 and resid 358 and name CA)	6.96	0.77	0.77
35	assign (segid 3A4 and resid 356 and name CA)	(segid 3A4 and resid 358 and name CB)	7.75	0.84	0.84
	assign (segid 3A4 and resid 356 and name CA)	(segid 3A4 and resid 358 and name N)	5.80	0.83	0.84
	assign (segid 3A4 and resid 356 and name CA)	(segid 3A4 and resid 359 and name CB)	9.74	0.44	0.45
	assign (segid 3A4 and resid 356 and name CA)	(segid 3A4 and resid 359 and name CA)	10.83	0.29	0.28
	assign (segid 3A4 and resid 356 and name CA)	(segid 3A4 and resid 360 and name CA)	8.54	0.31	0.30
40	assign (segid 3A4 and resid 356 and name CA)	(segid 3A4 and resid 360 and name CB)	7.79	0.29	0.29
	assign (segid 3A4 and resid 356 and name CA)	(segid 3A4 and resid 361 and name CA)	12.24	0.29	0.29
	assign (segid 3A4 and resid 356 and name CA)	(segid 3A4 and resid 361 and name CB)	13.07	0.30	0.30
	assign (segid 3A4 and resid 356 and name CA)	(segid 3A4 and resid 362 and name CA)	13.45	0.38	0.39
	assign (segid 3A4 and resid 356 and name CA)	(segid 3A4 and resid 362 and name CB)	13.38	0.42	0.42
45	assign (segid 3A4 and resid 356 and name CA)	(segid 3A4 and resid 363 and name CA)	14.71	0.43	0.43
	assign (segid 3A4 and resid 356 and name CA)	(segid 3A4 and resid 363 and name CB)	16.02	0.47	0.47
	assign (segid 3A4 and resid 356 and name CA)	(segid 3A4 and resid 364 and name CA)	14.36	0.46	0.46
	assign (segid 3A4 and resid 356 and name CA)	(segid 3A4 and resid 364 and name CB)	13.60	0.44	0.44
	assign (segid 3A4 and resid 356 and name CA)	(segid 3A4 and resid 365 and name CA)	15.62	0.80	0.80
50	assign (segid 3A4 and resid 356 and name CA)	(segid 3A4 and resid 365 and name CB)	17.11	0.82	0.81
	assign (segid 3A4 and resid 356 and name CA)	(segid 3A4 and resid 381 and name CA)	9.08	0.43	0.44
	assign (segid 3A4 and resid 356 and name CA)	(segid 3A4 and resid 382 and name CA)	11.67	0.60	0.61
	assign (segid 3A4 and resid 356 and name CA)	(segid 3A4 and resid 382 and name CB)	11.46	0.67	0.67
	assign (segid 3A4 and resid 356 and name CA)	(segid 3A4 and resid 383 and name CA)	14.22	0.56	0.56
55	assign (segid 3A4 and resid 356 and name CA)	(segid 3A4 and resid 384 and name CA)	16.91	0.63	0.62
	assign (segid 3A4 and resid 356 and name CA)	(segid 3A4 and resid 384 and name CB)	17.34	0.64	0.63
	assign (segid 3A4 and resid 356 and name CA)	(segid 3A4 and resid 385 and name CA)	16.27	0.76	0.76
	assign (segid 3A4 and resid 356 and name CA)	(segid 3A4 and resid 386 and name CA)	16.00	0.98	0.97
	assign (segid 3A4 and resid 356 and name CB)	(segid 3A4 and resid 357 and name C)	5.59	0.06	0.07
60	assign (segid 3A4 and resid 356 and name CB)	(segid 3A4 and resid 357 and name CA)	4.46	0.04	0.05
	assign (segid 3A4 and resid 356 and name CB)	(segid 3A4 and resid 357 and name CB)	4.91	0.05	0.06
	assign (segid 3A4 and resid 356 and name CB)	(segid 3A4 and resid 357 and name N)	3.17	0.06	0.07
	assign (segid 3A4 and resid 356 and name CB)	(segid 3A4 and resid 357 and name O)	6.09	0.25	0.24
	assign (segid 3A4 and resid 356 and name CB)	(segid 3A4 and resid 358 and name CA)	8.07	0.74	0.73
65	assign (segid 3A4 and resid 356 and name CB)	(segid 3A4 and resid 358 and name CB)	8.97	0.81	0.81
	assign (segid 3A4 and resid 356 and name CB)	(segid 3A4 and resid 359 and name CA)	10.54	0.44	0.43
	assign (segid 3A4 and resid 356 and name CB)	(segid 3A4 and resid 359 and name CB)	11.66	0.26	0.26
	assign (segid 3A4 and resid 356 and name CB)	(segid 3A4 and resid 360 and name CA)	8.78	0.33	0.34
	assign (segid 3A4 and resid 356 and name CB)	(segid 3A4 and resid 360 and name CB)	7.95	0.36	0.37
70	assign (segid 3A4 and resid 356 and name CB)	(segid 3A4 and resid 361 and name CA)	12.37	0.32	0.32
	assign (segid 3A4 and resid 356 and name CB)	(segid 3A4 and resid 361 and name CB)	13.23	0.32	0.33
	assign (segid 3A4 and resid 356 and name CB)	(segid 3A4 and resid 362 and name CA)	13.77	0.38	0.38
	assign (segid 3A4 and resid 356 and name CB)	(segid 3A4 and resid 362 and name CB)	13.85	0.40	0.40
	assign (segid 3A4 and resid 356 and name CB)	(segid 3A4 and resid 363 and name CA)	14.79	0.42	0.41
75	assign (segid 3A4 and resid 356 and name CB)	(segid 3A4 and resid 363 and name CB)	16.02	0.48	0.48
	assign (segid 3A4 and resid 356 and name CB)	(segid 3A4 and resid 364 and name CA)	14.63	0.42	0.43
	assign (segid 3A4 and resid 356 and name CB)	(segid 3A4 and resid 364 and name CB)	14.01	0.40	0.41
	assign (segid 3A4 and resid 356 and name CB)	(segid 3A4 and resid 365 and name CA)	15.70	0.75	0.75
	assign (segid 3A4 and resid 356 and name CB)	(segid 3A4 and resid 365 and name CB)	17.15	0.76	0.76
80	assign (segid 3A4 and resid 356 and name CB)	(segid 3A4 and resid 381 and name CA)	7.82	0.42	0.43
	assign (segid 3A4 and resid 356 and name CB)	(segid 3A4 and resid 382 and name CA)	10.22	0.60	0.61
	assign (segid 3A4 and resid 356 and name CB)	(segid 3A4 and resid 382 and name CB)	9.96	0.67	0.66
	assign (segid 3A4 and resid 356 and name CB)	(segid 3A4 and resid 383 and name CA)	12.88	0.59	0.58

	assign (segid 3A4 and resid 356 and name CB) (segid 3A4 and resid 384 and name CA)	15.51	0.62	0.61
	assign (segid 3A4 and resid 356 and name CB) (segid 3A4 and resid 384 and name CB)	15.97	0.61	0.62
	assign (segid 3A4 and resid 356 and name CB) (segid 3A4 and resid 385 and name CA)	14.77	0.76	0.75
	assign (segid 3A4 and resid 356 and name CB) (segid 3A4 and resid 386 and name CA)	14.52	0.95	0.95
5	assign (segid 3A4 and resid 356 and name CB) (segid 3A4 and resid 387 and name CA)	17.34	0.88	0.87
	assign (segid 3A4 and resid 356 and name CB) (segid 3A4 and resid 390 and name CB)	17.97	0.69	0.68
	assign (segid 3A4 and resid 356 and name N) (segid 3A4 and resid 356 and name C)	2.46	0.04	0.03
	assign (segid 3A4 and resid 356 and name N) (segid 3A4 and resid 356 and name CA)	1.46	0.01	0.00
	assign (segid 3A4 and resid 356 and name N) (segid 3A4 and resid 356 and name CB)	2.46	0.01	0.02
10	assign (segid 3A4 and resid 356 and name N) (segid 3A4 and resid 357 and name O)	3.50	0.03	0.04
	assign (segid 3A4 and resid 356 and name N) (segid 3A4 and resid 357 and name C)	4.76	0.07	0.07
	assign (segid 3A4 and resid 356 and name N) (segid 3A4 and resid 357 and name CA)	4.23	0.04	0.04
	assign (segid 3A4 and resid 356 and name N) (segid 3A4 and resid 357 and name CB)	5.16	0.06	0.07
	assign (segid 3A4 and resid 356 and name N) (segid 3A4 and resid 357 and name N)	2.81	0.05	0.05
15	assign (segid 3A4 and resid 356 and name N) (segid 3A4 and resid 357 and name O)	5.15	0.38	0.38
	assign (segid 3A4 and resid 356 and name N) (segid 3A4 and resid 358 and name N)	5.73	0.69	0.70
	assign (segid 3A4 and resid 356 and name O) (segid 3A4 and resid 356 and name CB)	3.26	0.05	0.06
	assign (segid 3A4 and resid 356 and name O) (segid 3A4 and resid 357 and name C)	3.84	0.21	0.20
	assign (segid 3A4 and resid 356 and name O) (segid 3A4 and resid 357 and name CA)	2.77	0.05	0.06
20	assign (segid 3A4 and resid 356 and name O) (segid 3A4 and resid 357 and name CB)	3.85	0.12	0.12
	assign (segid 3A4 and resid 356 and name O) (segid 3A4 and resid 357 and name N)	2.25	0.02	0.03
	assign (segid 3A4 and resid 356 and name O) (segid 3A4 and resid 357 and name O)	4.74	0.26	0.26
	assign (segid 3A4 and resid 356 and name O) (segid 3A4 and resid 358 and name N)	4.76	0.93	0.93
	assign (segid 3A4 and resid 357 and name C) (segid 3A4 and resid 357 and name CB)	2.49	0.05	0.04
25	assign (segid 3A4 and resid 357 and name C) (segid 3A4 and resid 357 and name O)	1.23	0.00	0.01
	assign (segid 3A4 and resid 357 and name C) (segid 3A4 and resid 358 and name C)	3.50	0.86	0.86
	assign (segid 3A4 and resid 357 and name C) (segid 3A4 and resid 358 and name CA)	2.95	0.91	0.90
	assign (segid 3A4 and resid 357 and name C) (segid 3A4 and resid 358 and name CB)	4.12	0.92	0.92
	assign (segid 3A4 and resid 357 and name C) (segid 3A4 and resid 358 and name N)	1.83	0.91	0.90
30	assign (segid 3A4 and resid 357 and name C) (segid 3A4 and resid 358 and name O)	3.92	1.04	1.04
	assign (segid 3A4 and resid 357 and name C) (segid 3A4 and resid 359 and name C)	4.98	0.47	0.46
	assign (segid 3A4 and resid 357 and name C) (segid 3A4 and resid 359 and name CA)	5.20	0.45	0.46
	assign (segid 3A4 and resid 357 and name C) (segid 3A4 and resid 359 and name CB)	6.17	0.25	0.26
	assign (segid 3A4 and resid 357 and name C) (segid 3A4 and resid 359 and name N)	4.16	0.52	0.52
35	assign (segid 3A4 and resid 357 and name C) (segid 3A4 and resid 359 and name O)	5.67	0.45	0.44
	assign (segid 3A4 and resid 357 and name C) (segid 3A4 and resid 360 and name C)	6.27	0.38	0.38
	assign (segid 3A4 and resid 357 and name C) (segid 3A4 and resid 360 and name CA)	4.81	0.39	0.39
	assign (segid 3A4 and resid 357 and name C) (segid 3A4 and resid 360 and name CB)	4.72	0.33	0.34
	assign (segid 3A4 and resid 357 and name C) (segid 3A4 and resid 360 and name N)	4.54	0.47	0.46
40	assign (segid 3A4 and resid 357 and name C) (segid 3A4 and resid 360 and name O)	6.82	0.34	0.34
	assign (segid 3A4 and resid 357 and name CA) (segid 3A4 and resid 357 and name C)	1.52	0.01	0.01
	assign (segid 3A4 and resid 357 and name CA) (segid 3A4 and resid 357 and name CB)	1.53	0.01	0.01
	assign (segid 3A4 and resid 357 and name CA) (segid 3A4 and resid 357 and name O)	2.39	0.01	0.02
	assign (segid 3A4 and resid 357 and name CA) (segid 3A4 and resid 358 and name C)	4.84	0.78	0.79
45	assign (segid 3A4 and resid 357 and name CA) (segid 3A4 and resid 358 and name CA)	4.29	0.86	0.85
	assign (segid 3A4 and resid 357 and name CA) (segid 3A4 and resid 358 and name CB)	5.29	0.97	0.96
	assign (segid 3A4 and resid 357 and name CA) (segid 3A4 and resid 358 and name N)	2.97	0.98	0.98
	assign (segid 3A4 and resid 357 and name CA) (segid 3A4 and resid 358 and name O)	5.04	1.00	1.01
	assign (segid 3A4 and resid 357 and name CA) (segid 3A4 and resid 359 and name C)	6.04	0.35	0.35
50	assign (segid 3A4 and resid 357 and name CA) (segid 3A4 and resid 359 and name CA)	6.50	0.37	0.36
	assign (segid 3A4 and resid 357 and name CA) (segid 3A4 and resid 359 and name CB)	7.44	0.20	0.20
	assign (segid 3A4 and resid 357 and name CA) (segid 3A4 and resid 359 and name N)	5.56	0.44	0.45
	assign (segid 3A4 and resid 357 and name CA) (segid 3A4 and resid 359 and name O)	6.57	0.35	0.34
	assign (segid 3A4 and resid 357 and name CA) (segid 3A4 and resid 360 and name C)	6.77	0.25	0.25
55	assign (segid 3A4 and resid 357 and name CA) (segid 3A4 and resid 360 and name CA)	5.39	0.26	0.27
	assign (segid 3A4 and resid 357 and name CA) (segid 3A4 and resid 360 and name CB)	5.20	0.24	0.24
	assign (segid 3A4 and resid 357 and name CA) (segid 3A4 and resid 360 and name N)	5.49	0.34	0.35
	assign (segid 3A4 and resid 357 and name CA) (segid 3A4 and resid 360 and name O)	7.09	0.22	0.22
	assign (segid 3A4 and resid 357 and name CA) (segid 3A4 and resid 361 and name CA)	9.14	0.26	0.26
60	assign (segid 3A4 and resid 357 and name CA) (segid 3A4 and resid 361 and name CB)	10.15	0.25	0.24
	assign (segid 3A4 and resid 357 and name CA) (segid 3A4 and resid 362 and name CA)	9.80	0.39	0.39
	assign (segid 3A4 and resid 357 and name CA) (segid 3A4 and resid 362 and name CB)	9.67	0.41	0.40
	assign (segid 3A4 and resid 357 and name CA) (segid 3A4 and resid 363 and name CA)	11.08	0.43	0.43
	assign (segid 3A4 and resid 357 and name CA) (segid 3A4 and resid 363 and name CB)	12.46	0.47	0.46
65	assign (segid 3A4 and resid 357 and name CA) (segid 3A4 and resid 364 and name CA)	10.72	0.44	0.44
	assign (segid 3A4 and resid 357 and name CA) (segid 3A4 and resid 364 and name CB)	9.92	0.42	0.41
	assign (segid 3A4 and resid 357 and name CA) (segid 3A4 and resid 365 and name CA)	12.40	0.73	0.73
	assign (segid 3A4 and resid 357 and name CA) (segid 3A4 and resid 365 and name CB)	13.91	0.73	0.73
	assign (segid 3A4 and resid 357 and name CA) (segid 3A4 and resid 381 and name CA)	9.21	0.42	0.42
70	assign (segid 3A4 and resid 357 and name CA) (segid 3A4 and resid 382 and name CA)	12.30	0.52	0.52
	assign (segid 3A4 and resid 357 and name CA) (segid 3A4 and resid 382 and name CB)	12.44	0.61	0.61
	assign (segid 3A4 and resid 357 and name CA) (segid 3A4 and resid 383 and name CA)	13.95	0.44	0.44
	assign (segid 3A4 and resid 357 and name CA) (segid 3A4 and resid 384 and name CA)	17.05	0.52	0.53
	assign (segid 3A4 and resid 357 and name CA) (segid 3A4 and resid 384 and name CB)	17.43	0.56	0.56
75	assign (segid 3A4 and resid 357 and name CA) (segid 3A4 and resid 385 and name CA)	17.18	0.64	0.63
	assign (segid 3A4 and resid 357 and name CA) (segid 3A4 and resid 386 and name CA)	17.61	0.83	0.83
	assign (segid 3A4 and resid 357 and name CB) (segid 3A4 and resid 358 and name C)	5.23	0.62	0.61
	assign (segid 3A4 and resid 357 and name CB) (segid 3A4 and resid 358 and name CA)	3.08	0.63	0.63
	assign (segid 3A4 and resid 357 and name CB) (segid 3A4 and resid 358 and name CB)	6.19	0.73	0.74
80	assign (segid 3A4 and resid 357 and name CB) (segid 3A4 and resid 358 and name N)	3.93	0.78	0.78
	assign (segid 3A4 and resid 357 and name CB) (segid 3A4 and resid 358 and name O)	5.20	0.87	0.86
	assign (segid 3A4 and resid 357 and name CB) (segid 3A4 and resid 359 and name C)	5.71	0.21	0.21
	assign (segid 3A4 and resid 357 and name CB) (segid 3A4 and resid 359 and name CA)	6.50	0.23	0.24

5	assign	(segid 3A4 and resid 357 and name CB)	(segid 3A4 and resid 359 and name CB)	7.48	0.14	0.13
	assign	(segid 3A4 and resid 357 and name CB)	(segid 3A4 and resid 359 and name N)	5.85	0.30	0.31
	assign	(segid 3A4 and resid 357 and name CB)	(segid 3A4 and resid 359 and name O)	6.07	0.23	0.22
	assign	(segid 3A4 and resid 357 and name CB)	(segid 3A4 and resid 360 and name C)	5.80	0.13	0.14
	assign	(segid 3A4 and resid 357 and name CB)	(segid 3A4 and resid 360 and name CA)	4.59	0.17	0.17
10	assign	(segid 3A4 and resid 357 and name CB)	(segid 3A4 and resid 360 and name CB)	4.44	0.22	0.23
	assign	(segid 3A4 and resid 357 and name CB)	(segid 3A4 and resid 360 and name N)	5.06	0.22	0.22
	assign	(segid 3A4 and resid 357 and name CB)	(segid 3A4 and resid 360 and name O)	5.93	0.13	0.12
	assign	(segid 3A4 and resid 357 and name CB)	(segid 3A4 and resid 361 and name CA)	8.21	0.13	0.14
	assign	(segid 3A4 and resid 357 and name CB)	(segid 3A4 and resid 361 and name CB)	9.32	0.11	0.11
15	assign	(segid 3A4 and resid 357 and name CB)	(segid 3A4 and resid 361 and name N)	6.96	0.15	0.15
	assign	(segid 3A4 and resid 357 and name CB)	(segid 3A4 and resid 362 and name CA)	9.00	0.29	0.28
	assign	(segid 3A4 and resid 357 and name CB)	(segid 3A4 and resid 362 and name CB)	9.08	0.30	0.29
	assign	(segid 3A4 and resid 357 and name CB)	(segid 3A4 and resid 363 and name CA)	10.04	0.40	0.40
	assign	(segid 3A4 and resid 357 and name CB)	(segid 3A4 and resid 363 and name CB)	11.35	0.45	0.45
20	assign	(segid 3A4 and resid 357 and name CB)	(segid 3A4 and resid 364 and name CA)	10.00	0.40	0.40
	assign	(segid 3A4 and resid 357 and name CB)	(segid 3A4 and resid 364 and name CB)	9.37	0.37	0.37
	assign	(segid 3A4 and resid 357 and name CB)	(segid 3A4 and resid 365 and name CA)	11.66	0.67	0.66
	assign	(segid 3A4 and resid 357 and name CB)	(segid 3A4 and resid 365 and name CB)	13.13	0.66	0.67
	assign	(segid 3A4 and resid 357 and name CB)	(segid 3A4 and resid 381 and name CA)	8.34	0.49	0.48
25	assign	(segid 3A4 and resid 357 and name CB)	(segid 3A4 and resid 382 and name CA)	11.37	0.56	0.56
	assign	(segid 3A4 and resid 357 and name CB)	(segid 3A4 and resid 382 and name CB)	11.59	0.66	0.66
	assign	(segid 3A4 and resid 357 and name CB)	(segid 3A4 and resid 383 and name CA)	12.73	0.49	0.49
	assign	(segid 3A4 and resid 357 and name CB)	(segid 3A4 and resid 384 and name CA)	15.96	0.57	0.57
	assign	(segid 3A4 and resid 357 and name CB)	(segid 3A4 and resid 384 and name CB)	16.38	0.61	0.60
30	assign	(segid 3A4 and resid 357 and name CB)	(segid 3A4 and resid 385 and name CA)	16.26	0.67	0.66
	assign	(segid 3A4 and resid 357 and name CB)	(segid 3A4 and resid 386 and name CA)	16.97	0.84	0.84
	assign	(segid 3A4 and resid 357 and name N)	(segid 3A4 and resid 357 and name C)	2.45	0.02	0.01
	assign	(segid 3A4 and resid 357 and name N)	(segid 3A4 and resid 357 and name CA)	1.46	0.01	0.02
	assign	(segid 3A4 and resid 357 and name N)	(segid 3A4 and resid 357 and name CB)	2.46	0.02	0.02
35	assign	(segid 3A4 and resid 357 and name N)	(segid 3A4 and resid 357 and name O)	3.10	0.22	0.23
	assign	(segid 3A4 and resid 357 and name N)	(segid 3A4 and resid 358 and name C)	5.79	0.69	0.69
	assign	(segid 3A4 and resid 357 and name N)	(segid 3A4 and resid 358 and name CA)	5.04	0.75	0.75
	assign	(segid 3A4 and resid 357 and name N)	(segid 3A4 and resid 358 and name N)	3.80	0.85	0.86
	assign	(segid 3A4 and resid 357 and name N)	(segid 3A4 and resid 359 and name C)	7.10	0.36	0.36
40	assign	(segid 3A4 and resid 357 and name N)	(segid 3A4 and resid 359 and name N)	6.49	0.44	0.43
	assign	(segid 3A4 and resid 357 and name N)	(segid 3A4 and resid 360 and name CA)	6.25	0.27	0.27
	assign	(segid 3A4 and resid 357 and name N)	(segid 3A4 and resid 360 and name CB)	5.72	0.24	0.24
	assign	(segid 3A4 and resid 357 and name O)	(segid 3A4 and resid 360 and name N)	6.39	0.36	0.35
	assign	(segid 3A4 and resid 357 and name O)	(segid 3A4 and resid 357 and name CB)	2.93	0.10	0.10
45	assign	(segid 3A4 and resid 357 and name O)	(segid 3A4 and resid 358 and name C)	3.44	0.84	0.84
	assign	(segid 3A4 and resid 357 and name O)	(segid 3A4 and resid 358 and name CA)	3.23	0.81	0.81
	assign	(segid 3A4 and resid 357 and name O)	(segid 3A4 and resid 358 and name CB)	4.57	0.76	0.77
	assign	(segid 3A4 and resid 357 and name O)	(segid 3A4 and resid 358 and name N)	2.59	0.62	0.62
	assign	(segid 3A4 and resid 357 and name O)	(segid 3A4 and resid 358 and name O)	3.96	1.04	1.05
50	assign	(segid 3A4 and resid 357 and name O)	(segid 3A4 and resid 359 and name C)	4.39	0.61	0.60
	assign	(segid 3A4 and resid 357 and name O)	(segid 3A4 and resid 359 and name CA)	4.66	0.51	0.51
	assign	(segid 3A4 and resid 357 and name O)	(segid 3A4 and resid 359 and name CB)	5.75	0.27	0.26
	assign	(segid 3A4 and resid 357 and name O)	(segid 3A4 and resid 359 and name N)	3.77	0.52	0.52
	assign	(segid 3A4 and resid 357 and name O)	(segid 3A4 and resid 359 and name O)	5.18	0.57	0.57
55	assign	(segid 3A4 and resid 357 and				

	assign (segid 3A4 and resid 358 and name CA)	(segid 3A4 and resid 360 and name CA)	5.40	0.07	0.07
	assign (segid 3A4 and resid 358 and name CA)	(segid 3A4 and resid 360 and name CB)	5.58	0.24	0.24
	assign (segid 3A4 and resid 358 and name CA)	(segid 3A4 and resid 360 and name N)	4.43	0.10	0.10
	assign (segid 3A4 and resid 358 and name CA)	(segid 3A4 and resid 360 and name O)	7.61	0.04	0.04
5	assign (segid 3A4 and resid 358 and name CA)	(segid 3A4 and resid 361 and name CA)	8.51	0.21	0.21
	assign (segid 3A4 and resid 358 and name CA)	(segid 3A4 and resid 361 and name CB)	9.15	0.41	0.41
	assign (segid 3A4 and resid 358 and name CA)	(segid 3A4 and resid 361 and name N)	7.14	0.20	0.20
	assign (segid 3A4 and resid 358 and name CA)	(segid 3A4 and resid 362 and name CA)	8.76	0.14	0.14
	assign (segid 3A4 and resid 358 and name CA)	(segid 3A4 and resid 362 and name CB)	8.12	0.17	0.17
10	assign (segid 3A4 and resid 358 and name CA)	(segid 3A4 and resid 363 and name CA)	11.13	0.39	0.38
	assign (segid 3A4 and resid 358 and name CA)	(segid 3A4 and resid 363 and name CB)	12.58	0.36	0.36
	assign (segid 3A4 and resid 358 and name CA)	(segid 3A4 and resid 364 and name CA)	10.74	0.52	0.52
	assign (segid 3A4 and resid 358 and name CA)	(segid 3A4 and resid 364 and name CB)	9.56	0.53	0.54
	assign (segid 3A4 and resid 358 and name CA)	(segid 3A4 and resid 365 and name CA)	13.32	0.77	0.77
	assign (segid 3A4 and resid 358 and name CA)	(segid 3A4 and resid 365 and name CB)	14.78	0.74	0.75
15	assign (segid 3A4 and resid 358 and name CA)	(segid 3A4 and resid 381 and name CA)	13.29	1.07	1.08
	assign (segid 3A4 and resid 358 and name CA)	(segid 3A4 and resid 382 and name CA)	16.33	1.07	1.08
	assign (segid 3A4 and resid 358 and name CA)	(segid 3A4 and resid 382 and name CB)	16.45	1.14	1.13
	assign (segid 3A4 and resid 358 and name CB)	(segid 3A4 and resid 359 and name C)	5.41	0.20	0.19
20	assign (segid 3A4 and resid 358 and name CB)	(segid 3A4 and resid 359 and name CB)	4.64	0.14	0.13
	assign (segid 3A4 and resid 358 and name CB)	(segid 3A4 and resid 359 and name N)	5.06	0.21	0.20
	assign (segid 3A4 and resid 358 and name CB)	(segid 3A4 and resid 359 and name O)	3.30	0.18	0.18
	assign (segid 3A4 and resid 358 and name CB)	(segid 3A4 and resid 360 and name CA)	6.13	0.35	0.36
	assign (segid 3A4 and resid 358 and name CB)	(segid 3A4 and resid 360 and name CB)	6.71	0.10	0.11
25	assign (segid 3A4 and resid 358 and name CB)	(segid 3A4 and resid 360 and name N)	7.02	0.25	0.24
	assign (segid 3A4 and resid 358 and name CB)	(segid 3A4 and resid 361 and name CA)	5.70	0.13	0.13
	assign (segid 3A4 and resid 358 and name CB)	(segid 3A4 and resid 361 and name CB)	9.62	0.26	0.25
	assign (segid 3A4 and resid 358 and name CB)	(segid 3A4 and resid 362 and name CA)	10.24	0.49	0.48
	assign (segid 3A4 and resid 358 and name CB)	(segid 3A4 and resid 362 and name CB)	9.43	0.33	0.34
30	assign (segid 3A4 and resid 358 and name CB)	(segid 3A4 and resid 363 and name CA)	8.61	0.38	0.38
	assign (segid 3A4 and resid 358 and name CB)	(segid 3A4 and resid 363 and name CB)	11.72	0.65	0.65
	assign (segid 3A4 and resid 358 and name CB)	(segid 3A4 and resid 364 and name CA)	13.19	0.60	0.61
	assign (segid 3A4 and resid 358 and name CB)	(segid 3A4 and resid 364 and name CB)	10.94	0.90	0.90
	assign (segid 3A4 and resid 358 and name CB)	(segid 3A4 and resid 365 and name CA)	9.66	0.93	0.92
35	assign (segid 3A4 and resid 358 and name CB)	(segid 3A4 and resid 365 and name CB)	13.46	1.20	1.20
	assign (segid 3A4 and resid 358 and name CB)	(segid 3A4 and resid 381 and name CA)	14.91	1.18	1.18
	assign (segid 3A4 and resid 358 and name CB)	(segid 3A4 and resid 381 and name CB)	14.24	1.24	1.23
	assign (segid 3A4 and resid 358 and name N)	(segid 3A4 and resid 358 and name C)	2.46	0.03	0.04
	assign (segid 3A4 and resid 358 and name N)	(segid 3A4 and resid 358 and name CA)	1.46	0.02	0.02
40	assign (segid 3A4 and resid 358 and name N)	(segid 3A4 and resid 358 and name CB)	2.39	0.05	0.05
	assign (segid 3A4 and resid 358 and name N)	(segid 3A4 and resid 359 and name C)	3.01	0.25	0.24
	assign (segid 3A4 and resid 358 and name N)	(segid 3A4 and resid 359 and name CB)	4.88	0.05	0.05
	assign (segid 3A4 and resid 358 and name N)	(segid 3A4 and resid 359 and name CA)	4.68	0.16	0.17
	assign (segid 3A4 and resid 358 and name N)	(segid 3A4 and resid 359 and name CB)	5.51	0.22	0.22
45	assign (segid 3A4 and resid 358 and name N)	(segid 3A4 and resid 359 and name N)	3.40	0.22	0.21
	assign (segid 3A4 and resid 358 and name N)	(segid 3A4 and resid 359 and name O)	5.63	0.15	0.15
	assign (segid 3A4 and resid 358 and name N)	(segid 3A4 and resid 360 and name C)	6.80	0.09	0.10
	assign (segid 3A4 and resid 358 and name N)	(segid 3A4 and resid 360 and name CA)	5.39	0.11	0.11
	assign (segid 3A4 and resid 358 and name N)	(segid 3A4 and resid 360 and name CB)	5.48	0.11	0.10
50	assign (segid 3A4 and resid 358 and name N)	(segid 3A4 and resid 360 and name N)	4.74	0.12	0.11
	assign (segid 3A4 and resid 358 and name N)	(segid 3A4 and resid 361 and name N)	7.44	0.11	0.12
	assign (segid 3A4 and resid 358 and name O)	(segid 3A4 and resid 358 and name CB)	3.23	0.17	0.17
	assign (segid 3A4 and resid 358 and name O)	(segid 3A4 and resid 359 and name C)	2.95	0.16	0.16
	assign (segid 3A4 and resid 358 and name O)	(segid 3A4 and resid 359 and name CA)	2.77	0.05	0.05
55	assign (segid 3A4 and resid 358 and name O)	(segid 3A4 and resid 359 and name CB)	3.46	0.38	0.38
	assign (segid 3A4 and resid 358 and name O)	(segid 3A4 and resid 359 and name N)	2.24	0.01	0.01
	assign (segid 3A4 and resid 358 and name O)	(segid 3A4 and resid 359 and name O)	3.56	0.48	0.48
	assign (segid 3A4 and resid 358 and name O)	(segid 3A4 and resid 360 and name C)	5.25	0.14	0.13
	assign (segid 3A4 and resid 358 and name O)	(segid 3A4 and resid 360 and name CB)	4.17	0.11	0.12
60	assign (segid 3A4 and resid 358 and name O)	(segid 3A4 and resid 360 and name N)	4.76	0.40	0.40
	assign (segid 3A4 and resid 358 and name O)	(segid 3A4 and resid 360 and name O)	3.25	0.21	0.20
	assign (segid 3A4 and resid 358 and name O)	(segid 3A4 and resid 361 and name C)	6.08	0.20	0.21
	assign (segid 3A4 and resid 358 and name O)	(segid 3A4 and resid 361 and name CA)	7.04	0.21	0.22
	assign (segid 3A4 and resid 358 and name O)	(segid 3A4 and resid 361 and name N)	6.81	0.34	0.35
65	assign (segid 3A4 and resid 358 and name O)	(segid 3A4 and resid 362 and name CA)	5.56	0.34	0.34
	assign (segid 3A4 and resid 358 and name O)	(segid 3A4 and resid 362 and name CB)	6.85	0.39	0.39
	assign (segid 3A4 and resid 358 and name O)	(segid 3A4 and resid 362 and name N)	6.27	0.47	0.47
	assign (segid 3A4 and resid 358 and name O)	(segid 3A4 and resid 362 and name O)	6.23	0.22	0.23
	assign (segid 3A4 and resid 359 and name C)	(segid 3A4 and resid 359 and name CB)	2.50	0.02	0.03
70	assign (segid 3A4 and resid 359 and name C)	(segid 3A4 and resid 360 and name C)	1.23	0.00	0.01
	assign (segid 3A4 and resid 359 and name C)	(segid 3A4 and resid 360 and name CA)	3.12	0.01	0.02
	assign (segid 3A4 and resid 359 and name C)	(segid 3A4 and resid 360 and name CB)	2.49	0.02	0.02
	assign (segid 3A4 and resid 359 and name C)	(segid 3A4 and resid 360 and name N)	3.65	0.03	0.04
	assign (segid 3A4 and resid 359 and name C)	(segid 3A4 and resid 360 and name O)	1.35	0.01	0.01
75	assign (segid 3A4 and resid 359 and name C)	(segid 3A4 and resid 361 and name C)	4.13	0.03	0.03
	assign (segid 3A4 and resid 359 and name C)	(segid 3A4 and resid 361 and name CA)	4.62	0.10	0.09
	assign (segid 3A4 and resid 359 and name C)	(segid 3A4 and resid 361 and name CB)	4.41	0.07	0.08
	assign (segid 3A4 and resid 359 and name C)	(segid 3A4 and resid 361 and name N)	5.21	0.13	0.12
	assign (segid 3A4 and resid 359 and name C)	(segid 3A4 and resid 361 and name O)	3.19	0.08	0.07
80	assign (segid 3A4 and resid 359 and name C)	(segid 3A4 and resid 362 and name C)	5.80	0.11	0.10
	assign (segid 3A4 and resid 359 and name C)	(segid 3A4 and resid 362 and name CA)	5.38	0.10	0.09
	assign (segid 3A4 and resid 359 and name C)	(segid 3A4 and resid 362 and name CB)	4.72	0.09	0.09
	assign (segid 3A4 and resid 359 and name C)	(segid 3A4 and resid 362 and name N)	4.41	0.13	0.13

	assign (segid 3A4 and resid 359 and name C) (segid 3A4 and resid 362 and name N)	3.85	0.08	0.09
	assign (segid 3A4 and resid 359 and name C) (segid 3A4 and resid 362 and name O)	4.96	0.12	0.12
	assign (segid 3A4 and resid 359 and name C) (segid 3A4 and resid 363 and name CA)	7.64	0.11	0.10
	assign (segid 3A4 and resid 359 and name C) (segid 3A4 and resid 363 and name N)	6.69	0.10	0.10
5	assign (segid 3A4 and resid 359 and name C) (segid 3A4 and resid 364 and name CB)	7.54	0.25	0.25
	assign (segid 3A4 and resid 359 and name CA) (segid 3A4 and resid 359 and name C)	1.53	0.01	0.01
	assign (segid 3A4 and resid 359 and name CA) (segid 3A4 and resid 359 and name CB)	1.53	0.01	0.02
	assign (segid 3A4 and resid 359 and name CA) (segid 3A4 and resid 359 and name O)	2.41	0.01	0.01
	assign (segid 3A4 and resid 359 and name CA) (segid 3A4 and resid 360 and name C)	4.56	0.02	0.02
10	assign (segid 3A4 and resid 359 and name CA) (segid 3A4 and resid 360 and name CA)	3.84	0.02	0.02
	assign (segid 3A4 and resid 359 and name CA) (segid 3A4 and resid 360 and name CB)	4.72	0.04	0.04
	assign (segid 3A4 and resid 359 and name CA) (segid 3A4 and resid 360 and name N)	2.44	0.00	0.01
	assign (segid 3A4 and resid 359 and name CA) (segid 3A4 and resid 360 and name O)	5.63	0.04	0.03
	assign (segid 3A4 and resid 359 and name CA) (segid 3A4 and resid 361 and name C)	5.70	0.10	0.10
15	assign (segid 3A4 and resid 359 and name CA) (segid 3A4 and resid 361 and name CA)	5.55	0.09	0.09
	assign (segid 3A4 and resid 359 and name CA) (segid 3A4 and resid 361 and name CB)	6.07	0.16	0.15
	assign (segid 3A4 and resid 359 and name CA) (segid 3A4 and resid 361 and name N)	4.40	0.08	0.08
	assign (segid 3A4 and resid 359 and name CA) (segid 3A4 and resid 361 and name O)	6.83	0.13	0.13
	assign (segid 3A4 and resid 359 and name CA) (segid 3A4 and resid 362 and name C)	6.43	0.13	0.12
20	assign (segid 3A4 and resid 359 and name CA) (segid 3A4 and resid 362 and name CA)	5.61	0.11	0.10
	assign (segid 3A4 and resid 359 and name CA) (segid 3A4 and resid 362 and name CB)	4.94	0.17	0.17
	assign (segid 3A4 and resid 359 and name CA) (segid 3A4 and resid 362 and name N)	4.92	0.09	0.08
	assign (segid 3A4 and resid 359 and name CA) (segid 3A4 and resid 362 and name O)	6.13	0.14	0.14
	assign (segid 3A4 and resid 359 and name CA) (segid 3A4 and resid 363 and name CA)	8.72	0.15	0.14
25	assign (segid 3A4 and resid 359 and name CA) (segid 3A4 and resid 363 and name CB)	10.07	0.13	0.14
	assign (segid 3A4 and resid 359 and name CA) (segid 3A4 and resid 363 and name N)	7.70	0.14	0.14
	assign (segid 3A4 and resid 359 and name CA) (segid 3A4 and resid 364 and name CA)	9.18	0.28	0.28
	assign (segid 3A4 and resid 359 and name CA) (segid 3A4 and resid 364 and name CB)	8.11	0.30	0.30
	assign (segid 3A4 and resid 359 and name CA) (segid 3A4 and resid 365 and name CA)	12.46	0.39	0.38
30	assign (segid 3A4 and resid 359 and name CA) (segid 3A4 and resid 365 and name CB)	13.78	0.37	0.38
	assign (segid 3A4 and resid 359 and name CA) (segid 3A4 and resid 381 and name CA)	14.44	0.64	0.63
	assign (segid 3A4 and resid 359 and name CA) (segid 3A4 and resid 382 and name CA)	17.24	0.66	0.67
	assign (segid 3A4 and resid 359 and name CA) (segid 3A4 and resid 382 and name CB)	17.46	0.80	0.79
	assign (segid 3A4 and resid 359 and name CA) (segid 3A4 and resid 383 and name CA)	17.85	0.56	0.56
35	assign (segid 3A4 and resid 359 and name CB) (segid 3A4 and resid 360 and name C)	5.46	0.07	0.08
	assign (segid 3A4 and resid 359 and name CB) (segid 3A4 and resid 360 and name CA)	4.98	0.04	0.03
	assign (segid 3A4 and resid 359 and name CB) (segid 3A4 and resid 360 and name CB)	6.05	0.05	0.06
	assign (segid 3A4 and resid 359 and name CB) (segid 3A4 and resid 360 and name N)	3.73	0.03	0.03
	assign (segid 3A4 and resid 359 and name CB) (segid 3A4 and resid 360 and name O)	6.40	0.07	0.07
40	assign (segid 3A4 and resid 359 and name CB) (segid 3A4 and resid 361 and name C)	5.92	0.20	0.20
	assign (segid 3A4 and resid 359 and name CB) (segid 3A4 and resid 361 and name CA)	6.13	0.20	0.21
	assign (segid 3A4 and resid 359 and name CB) (segid 3A4 and resid 361 and name CB)	6.67	0.29	0.28
	assign (segid 3A4 and resid 359 and name CB) (segid 3A4 and resid 361 and name N)	5.22	0.16	0.16
	assign (segid 3A4 and resid 359 and name CB) (segid 3A4 and resid 361 and name O)	6.92	0.24	0.24
45	assign (segid 3A4 and resid 359 and name CB) (segid 3A4 and resid 362 and name C)	6.11	0.12	0.12
	assign (segid 3A4 and resid 359 and name CB) (segid 3A4 and resid 362 and name CA)	5.27	0.12	0.12
	assign (segid 3A4 and resid 359 and name CB) (segid 3A4 and resid 362 and name CB)	4.26	0.14	0.14
	assign (segid 3A4 and resid 359 and name CB) (segid 3A4 and resid 362 and name N)	4.95	0.14	0.14
	assign (segid 3A4 and resid 359 and name CB) (segid 3A4 and resid 362 and name O)	5.95	0.13	0.14
50	assign (segid 3A4 and resid 359 and name CB) (segid 3A4 and resid 363 and name CA)	8.34	0.17	0.17
	assign (segid 3A4 and resid 359 and name CB) (segid 3A4 and resid 363 and name CB)	9.70	0.15	0.15
	assign (segid 3A4 and resid 359 and name CB) (segid 3A4 and resid 363 and name N)	7.30	0.14	0.14
	assign (segid 3A4 and resid 359 and name CB) (segid 3A4 and resid 364 and name CA)	8.48	0.32	0.31
	assign (segid 3A4 and resid 359 and name CB) (segid 3A4 and resid 364 and name CB)	7.31	0.33	0.32
55	assign (segid 3A4 and resid 359 and name CB) (segid 3A4 and resid 365 and name CA)	11.89	0.34	0.35
	assign (segid 3A4 and resid 359 and name CB) (segid 3A4 and resid 365 and name CB)	13.18	0.36	0.35
	assign (segid 3A4 and resid 359 and name CB) (segid 3A4 and resid 381 and name CA)	15.29	0.59	0.58
	assign (segid 3A4 and resid 359 and name CB) (segid 3A4 and resid 382 and name CA)	18.22	0.56	0.57
	assign (segid 3A4 and resid 359 and name CB) (segid 3A4 and resid 383 and name CA)	18.70	0.48	0.48
60	assign (segid 3A4 and resid 359 and name N) (segid 3A4 and resid 359 and name C)	2.44	0.05	0.04
	assign (segid 3A4 and resid 359 and name N) (segid 3A4 and resid 359 and name CA)	1.46	0.00	0.01
	assign (segid 3A4 and resid 359 and name N) (segid 3A4 and resid 359 and name CB)	2.46	0.02	0.02
	assign (segid 3A4 and resid 359 and name N) (segid 3A4 and resid 359 and name O)	3.40	0.11	0.11
	assign (segid 3A4 and resid 359 and name N) (segid 3A4 and resid 360 and name C)	5.33	0.04	0.03
65	assign (segid 3A4 and resid 359 and name N) (segid 3A4 and resid 360 and name CA)	4.26	0.06	0.05
	assign (segid 3A4 and resid 359 and name N) (segid 3A4 and resid 360 and name CB)	4.85	0.13	0.13
	assign (segid 3A4 and resid 359 and name N) (segid 3A4 and resid 360 and name N)	2.91	0.07	0.08
	assign (segid 3A4 and resid 359 and name N) (segid 3A4 and resid 360 and name O)	6.35	0.02	0.02
	assign (segid 3A4 and resid 359 and name N) (segid 3A4 and resid 361 and name C)	6.96	0.13	0.12
70	assign (segid 3A4 and resid 359 and name N) (segid 3A4 and resid 361 and name CA)	6.69	0.10	0.11
	assign (segid 3A4 and resid 359 and name N) (segid 3A4 and resid 361 and name CB)	7.25	0.19	0.19
	assign (segid 3A4 and resid 359 and name N) (segid 3A4 and resid 361 and name N)	5.41	0.10	0.10
	assign (segid 3A4 and resid 359 and name N) (segid 3A4 and resid 362 and name C)	7.49	0.22	0.21
	assign (segid 3A4 and resid 359 and name N) (segid 3A4 and resid 362 and name CA)	6.84	0.18	0.17
75	assign (segid 3A4 and resid 359 and name N) (segid 3A4 and resid 362 and name CB)	6.15	0.21	0.22
	assign (segid 3A4 and resid 359 and name N) (segid 3A4 and resid 362 and name N)	6.16	0.13	0.13
	assign (segid 3A4 and resid 359 and name N) (segid 3A4 and resid 362 and name O)	7.02	0.26	0.26
	assign (segid 3A4 and resid 359 and name N) (segid 3A4 and resid 359 and name CB)	2.74	0.05	0.04
	assign (segid 3A4 and resid 359 and name N) (segid 3A4 and resid 360 and name C)	3.02	0.02	0.02
80	assign (segid 3A4 and resid 359 and name N) (segid 3A4 and resid 360 and name CA)	2.85	0.03	0.03
	assign (segid 3A4 and resid 359 and name N) (segid 3A4 and resid 360 and name CB)	4.29	0.05	0.04
	assign (segid 3A4 and resid 359 and name N) (segid 3A4 and resid 360 and name N)	2.26	0.01	0.01
	assign (segid 3A4 and resid 359 and name N) (segid 3A4 and resid 360 and name O)	3.78	0.06	0.05

	assign (segid 3A4 and resid 359 and name O) (segid 3A4 and resid 361 and name C)	3.93	0.13	0.13
	assign (segid 3A4 and resid 359 and name O) (segid 3A4 and resid 361 and name CA)	4.10	0.11	0.10
	assign (segid 3A4 and resid 359 and name O) (segid 3A4 and resid 361 and name CB)	5.10	0.16	0.15
	assign (segid 3A4 and resid 359 and name O) (segid 3A4 and resid 361 and name N)	3.12	0.09	0.09
5	assign (segid 3A4 and resid 359 and name O) (segid 3A4 and resid 362 and name O)	5.06	0.13	0.13
	assign (segid 3A4 and resid 359 and name O) (segid 3A4 and resid 362 and name C)	4.18	0.10	0.10
	assign (segid 3A4 and resid 359 and name O) (segid 3A4 and resid 362 and name CA)	3.63	0.09	0.10
	assign (segid 3A4 and resid 359 and name O) (segid 3A4 and resid 362 and name CB)	3.36	0.09	0.10
	assign (segid 3A4 and resid 359 and name O) (segid 3A4 and resid 362 and name N)	2.95	0.12	0.11
10	assign (segid 3A4 and resid 359 and name O) (segid 3A4 and resid 362 and name O)	3.78	0.13	0.13
	assign (segid 3A4 and resid 359 and name O) (segid 3A4 and resid 362 and name C)	6.71	0.14	0.14
	assign (segid 3A4 and resid 359 and name O) (segid 3A4 and resid 363 and name CA)	6.44	0.12	0.11
	assign (segid 3A4 and resid 359 and name O) (segid 3A4 and resid 363 and name N)	5.50	0.10	0.09
	assign (segid 3A4 and resid 359 and name O) (segid 3A4 and resid 363 and name O)	7.36	0.14	0.13
15	assign (segid 3A4 and resid 359 and name O) (segid 3A4 and resid 364 and name CA)	7.29	0.23	0.23
	assign (segid 3A4 and resid 359 and name O) (segid 3A4 and resid 364 and name CB)	6.48	0.24	0.23
	assign (segid 3A4 and resid 359 and name O) (segid 3A4 and resid 364 and name N)	6.60	0.20	0.21
	assign (segid 3A4 and resid 359 and name O) (segid 3A4 and resid 364 and name O)	6.61	0.46	0.47
	assign (segid 3A4 and resid 35 and name C) (segid 3A4 and resid 349 and name C)	6.05	0.27	0.26
20	assign (segid 3A4 and resid 35 and name C) (segid 3A4 and resid 349 and name CA)	7.01	0.39	0.38
	assign (segid 3A4 and resid 35 and name C) (segid 3A4 and resid 349 and name CB)	6.52	0.53	0.54
	assign (segid 3A4 and resid 35 and name C) (segid 3A4 and resid 349 and name O)	6.02	0.26	0.26
	assign (segid 3A4 and resid 35 and name C) (segid 3A4 and resid 350 and name C)	6.11	0.54	0.54
	assign (segid 3A4 and resid 35 and name C) (segid 3A4 and resid 350 and name CA)	5.02	0.45	0.46
25	assign (segid 3A4 and resid 35 and name C) (segid 3A4 and resid 350 and name CB)	5.09	0.57	0.57
	assign (segid 3A4 and resid 35 and name C) (segid 3A4 and resid 350 and name N)	5.60	0.30	0.31
	assign (segid 3A4 and resid 35 and name C) (segid 3A4 and resid 350 and name O)	6.11	0.66	0.67
	assign (segid 3A4 and resid 35 and name C) (segid 3A4 and resid 353 and name CB)	5.57	0.73	0.73
	assign (segid 3A4 and resid 35 and name C) (segid 3A4 and resid 353 and name CG)	5.21	0.80	0.79
30	assign (segid 3A4 and resid 35 and name C) (segid 3A4 and resid 35 and name O)	1.23	0.00	0.01
	assign (segid 3A4 and resid 35 and name C) (segid 3A4 and resid 36 and name C)	2.99	0.03	0.03
	assign (segid 3A4 and resid 35 and name C) (segid 3A4 and resid 36 and name CA)	2.43	0.02	0.02
	assign (segid 3A4 and resid 35 and name C) (segid 3A4 and resid 36 and name N)	1.33	0.00	0.00
	assign (segid 3A4 and resid 35 and name C) (segid 3A4 and resid 36 and name O)	3.85	0.08	0.08
35	assign (segid 3A4 and resid 35 and name C) (segid 3A4 and resid 37 and name C)	4.57	0.10	0.10
	assign (segid 3A4 and resid 35 and name C) (segid 3A4 and resid 37 and name CA)	4.41	0.10	0.10
	assign (segid 3A4 and resid 35 and name C) (segid 3A4 and resid 37 and name CB)	5.05	0.20	0.20
	assign (segid 3A4 and resid 35 and name C) (segid 3A4 and resid 37 and name N)	3.23	0.11	0.10
	assign (segid 3A4 and resid 35 and name C) (segid 3A4 and resid 37 and name O)	5.66	0.11	0.11
40	assign (segid 3A4 and resid 35 and name C) (segid 3A4 and resid 38 and name C)	4.95	0.10	0.11
	assign (segid 3A4 and resid 35 and name C) (segid 3A4 and resid 38 and name CA)	4.66	0.14	0.14
	assign (segid 3A4 and resid 35 and name C) (segid 3A4 and resid 38 and name CB)	4.58	0.23	0.24
	assign (segid 3A4 and resid 35 and name C) (segid 3A4 and resid 38 and name N)	3.88	0.12	0.11
	assign (segid 3A4 and resid 35 and name C) (segid 3A4 and resid 38 and name O)	6.15	0.10	0.10
45	assign (segid 3A4 and resid 35 and name C) (segid 3A4 and resid 39 and name C)	6.06	0.12	0.12
	assign (segid 3A4 and resid 35 and name C) (segid 3A4 and resid 39 and name CA)	5.02	0.12	0.12
	assign (segid 3A4 and resid 35 and name C) (segid 3A4 and resid 39 and name CB)	4.55	0.18	0.19
	assign (segid 3A4 and resid 35 and name C) (segid 3A4 and resid 39 and name N)	4.16	0.09	0.09
	assign (segid 3A4 and resid 35 and name C) (segid 3A4 and resid 39 and name O)	7.22	0.12	0.12
50	assign (segid 3A4 and resid 35 and name C) (segid 3A4 and resid 40 and name CA)	7.24	0.11	0.12
	assign (segid 3A4 and resid 35 and name C) (segid 3A4 and resid 40 and name CB)	7.33	0.12	0.12
	assign (segid 3A4 and resid 35 and name C) (segid 3A4 and resid 40 and name N)	5.95	0.11	0.12
	assign (segid 3A4 and resid 35 and name C) (segid 3A4 and resid 41 and name N)	7.78	0.09	0.09
	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 313 and name CA)	17.60	0.58	0.58
55	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 313 and name CB)	17.87	0.52	0.52
	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 314 and name CA)	14.52	0.58	0.58
	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 314 and name CB)	14.51	0.55	0.55
	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 315 and name CA)	15.59	0.75	0.75
	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 315 and name CB)	16.88	0.75	0.75
60	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 316 and name CA)	16.83	0.87	0.86
	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 317 and name CA)	14.87	0.44	0.44
	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 318 and name CA)	17.45	0.81	0.81
	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 318 and name CB)	18.71	0.72	0.72
	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 319 and name CA)	16.11	0.69	0.69
65	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 319 and name CB)	16.39	0.79	0.79
	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 322 and name CA)	15.08	0.79	0.80
	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 323 and name CA)	15.75	0.35	0.35
	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 323 and name CB)	14.76	0.40	0.39
	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 324 and name CA)	17.98	0.20	0.20
70	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 324 and name CB)	19.43	0.18	0.18
	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 325 and name CA)	18.11	0.25	0.24
	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 325 and name CB)	17.68	0.25	0.26
	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 329 and name CA)	17.46	0.87	0.88
	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 329 and name CB)	16.73	0.83	0.83
75	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 330 and name CA)	15.54	1.08	1.09
	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 330 and name CB)	16.42	1.16	1.17
	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 331 and name CA)	11.80	1.10	1.11
	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 331 and name CB)	11.10	1.07	1.07
	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 332 and name CA)	10.68	1.23	1.23
80	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 333 and name CA)	13.87	1.03	1.03
	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 335 and name CA)	13.90	0.89	0.89
	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 336 and name CA)	16.57	0.77	0.76
	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 336 and name CB)	17.95	0.77	0.76

	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 337 and name CA)	16.38	0.78	0.78
	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 337 and name CB)	15.34	0.73	0.73
	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 341 and name CA)	18.58	0.33	0.33
	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 341 and name CB)	17.74	0.42	0.42
	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 342 and name CA)	16.81	0.25	0.24
5	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 343 and name CA)	13.10	0.29	0.29
	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 343 and name CB)	12.53	0.39	0.39
	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 344 and name CA)	11.71	0.19	0.19
	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 344 and name CB)	12.19	0.35	0.34
	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 345 and name CA)	8.95	0.15	0.16
10	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 345 and name CB)	9.24	0.26	0.27
	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 346 and name CA)	8.38	0.35	0.34
	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 346 and name CB)	7.99	0.44	0.45
	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 346 and name O)	6.96	0.33	0.33
	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 347 and name CA)	9.11	0.33	0.33
15	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 347 and name CB)	10.51	0.37	0.38
	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 348 and name CA)	10.05	0.18	0.17
	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 349 and name C)	6.09	0.17	0.17
	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 349 and name CA)	6.88	0.17	0.18
	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 349 and name CB)	6.20	0.32	0.32
20	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 349 and name O)	5.96	0.18	0.17
	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 350 and name CA)	5.62	0.57	0.56
	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 350 and name CB)	6.00	0.63	0.62
	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 350 and name N)	5.94	0.37	0.36
	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 351 and name CA)	9.07	0.63	0.63
25	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 352 and name CA)	9.09	0.64	0.64
	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 352 and name CB)	9.59	0.63	0.62
	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 353 and name CA)	6.65	0.76	0.76
	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 353 and name CB)	5.59	0.90	0.90
	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 353 and name CG)	5.05	0.98	0.99
30	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 354 and name CA)	9.62	0.70	0.70
	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 354 and name CB)	10.21	0.63	0.62
	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 355 and name CA)	9.20	1.03	1.04
	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 355 and name CB)	8.33	1.12	1.13
	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 356 and name CA)	9.71	0.91	0.92
35	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 356 and name CB)	8.80	0.87	0.87
	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 357 and name CA)	11.98	0.85	0.86
	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 357 and name CB)	11.84	0.86	0.86
	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 358 and name CA)	14.47	0.61	0.61
	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 358 and name CB)	15.67	0.68	0.68
40	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 359 and name CA)	15.79	0.63	0.64
	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 359 and name CB)	17.24	0.60	0.60
	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 35 and name C)	1.51	0.01	0.01
	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 35 and name O)	2.38	0.02	0.02
	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 360 and name CA)	13.27	0.59	0.59
45	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 360 and name CB)	11.82	0.60	0.60
	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 361 and name CA)	15.53	0.56	0.57
	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 361 and name CB)	15.77	0.57	0.57
	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 36 and name C)	4.38	0.04	0.04
	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 36 and name CA)	3.79	0.01	0.02
50	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 36 and name N)	2.43	0.03	0.03
	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 36 and name O)	5.30	0.08	0.08
	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 37 and name C)	5.53	0.13	0.14
	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 37 and name CA)	5.40	0.15	0.14
	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 37 and name CB)	5.69	0.28	0.28
55	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 37 and name N)	4.33	0.12	0.12
	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 37 and name O)	6.68	0.14	0.14
	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 381 and name CA)	11.97	0.72	0.72
	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 382 and name CA)	11.51	0.56	0.56
60	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 382 and name CB)	10.27	0.58	0.58
	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 383 and name CA)	14.02	0.46	0.45
	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 384 and name CA)	16.32	0.43	0.44
	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 384 and name CB)	17.39	0.42	0.42
	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 385 and name CA)	14.04	0.56	0.56
65	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 386 and name CA)	13.98	0.57	0.57
	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 387 and name CA)	16.22	0.81	0.81
	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 389 and name CB)	18.63	0.51	0.51
	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 38 and name C)	5.82	0.16	0.15
	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 38 and name CA)	5.30	0.22	0.22
	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 38 and name CB)	4.81	0.32	0.33
70	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 38 and name N)	4.66	0.17	0.17
	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 38 and name O)	6.98	0.16	0.16
	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 390 and name CA)	18.16	0.51	0.50
	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 390 and name CB)	18.15	0.56	0.57
	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 39 and name C)	7.32	0.12	0.12
75	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 39 and name CA)	6.15	0.13	0.13
	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 39 and name CB)	5.73	0.21	0.21
	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 39 and name N)	5.22	0.12	0.11
	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 40 and name CA)	8.64	0.10	0.10
	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 40 and name CB)	8.76	0.10	0.11
80	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 40 and name N)	7.32	0.11	0.12
	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 41 and name CA)	9.93	0.16	0.15
	assign (segid 3A4 and resid 35 and name CA) (segid 3A4 and resid 41 and name CB)	9.49	0.24	0.24

	assign (segid 3A4 and resid 35 and name CA)	(segid 3A4 and resid 42 and name CA)	10.60	0.14	0.14
	assign (segid 3A4 and resid 35 and name CA)	(segid 3A4 and resid 42 and name CB)	9.83	0.16	0.15
	assign (segid 3A4 and resid 35 and name N)	(segid 3A4 and resid 346 and name CB)	6.95	0.42	0.42
	assign (segid 3A4 and resid 35 and name N)	(segid 3A4 and resid 346 and name N)	7.07	0.23	0.23
5	assign (segid 3A4 and resid 35 and name N)	(segid 3A4 and resid 346 and name O)	6.35	0.33	0.33
	assign (segid 3A4 and resid 35 and name N)	(segid 3A4 and resid 349 and name C)	6.04	0.30	0.30
	assign (segid 3A4 and resid 35 and name N)	(segid 3A4 and resid 349 and name CA)	6.55	0.13	0.14
	assign (segid 3A4 and resid 35 and name N)	(segid 3A4 and resid 349 and name CB)	5.62	0.18	0.18
	assign (segid 3A4 and resid 35 and name N)	(segid 3A4 and resid 349 and name N)	7.51	0.15	0.15
10	assign (segid 3A4 and resid 35 and name N)	(segid 3A4 and resid 349 and name O)	6.12	0.26	0.26
	assign (segid 3A4 and resid 35 and name N)	(segid 3A4 and resid 350 and name CA)	5.92	0.72	0.71
	assign (segid 3A4 and resid 35 and name N)	(segid 3A4 and resid 350 and name CB)	6.26	0.79	0.79
	assign (segid 3A4 and resid 35 and name N)	(segid 3A4 and resid 350 and name N)	5.93	0.54	0.54
	assign (segid 3A4 and resid 35 and name N)	(segid 3A4 and resid 35 and name C)	2.45	0.03	0.03
15	assign (segid 3A4 and resid 35 and name N)	(segid 3A4 and resid 35 and name CA)	1.45	0.01	0.01
	assign (segid 3A4 and resid 35 and name N)	(segid 3A4 and resid 35 and name O)	2.76	0.08	0.08
	assign (segid 3A4 and resid 35 and name N)	(segid 3A4 and resid 36 and name C)	5.37	0.08	0.07
	assign (segid 3A4 and resid 35 and name N)	(segid 3A4 and resid 36 and name CA)	4.82	0.03	0.04
	assign (segid 3A4 and resid 35 and name N)	(segid 3A4 and resid 36 and name N)	3.61	0.04	0.03
20	assign (segid 3A4 and resid 35 and name N)	(segid 3A4 and resid 36 and name O)	6.09	0.10	0.10
	assign (segid 3A4 and resid 35 and name N)	(segid 3A4 and resid 37 and name C)	6.24	0.19	0.19
	assign (segid 3A4 and resid 35 and name N)	(segid 3A4 and resid 37 and name CA)	6.40	0.19	0.20
	assign (segid 3A4 and resid 35 and name N)	(segid 3A4 and resid 37 and name CB)	6.78	0.33	0.33
	assign (segid 3A4 and resid 35 and name N)	(segid 3A4 and resid 37 and name N)	5.45	0.15	0.16
25	assign (segid 3A4 and resid 35 and name N)	(segid 3A4 and resid 37 and name O)	7.29	0.20	0.21
	assign (segid 3A4 and resid 35 and name N)	(segid 3A4 and resid 38 and name C)	5.80	0.16	0.17
	assign (segid 3A4 and resid 35 and name N)	(segid 3A4 and resid 38 and name CA)	5.44	0.24	0.25
	assign (segid 3A4 and resid 35 and name N)	(segid 3A4 and resid 38 and name CB)	4.67	0.35	0.35
	assign (segid 3A4 and resid 35 and name N)	(segid 3A4 and resid 38 and name N)	5.17	0.21	0.22
30	assign (segid 3A4 and resid 35 and name N)	(segid 3A4 and resid 38 and name O)	6.86	0.17	0.17
	assign (segid 3A4 and resid 35 and name N)	(segid 3A4 and resid 39 and name C)	7.39	0.13	0.12
	assign (segid 3A4 and resid 35 and name N)	(segid 3A4 and resid 39 and name CA)	6.04	0.13	0.12
	assign (segid 3A4 and resid 35 and name N)	(segid 3A4 and resid 39 and name CB)	5.62	0.23	0.23
	assign (segid 3A4 and resid 35 and name N)	(segid 3A4 and resid 39 and name N)	5.23	0.09	0.09
35	assign (segid 3A4 and resid 35 and name N)	(segid 3A4 and resid 40 and name N)	7.64	0.12	0.12
	assign (segid 3A4 and resid 35 and name O)	(segid 3A4 and resid 346 and name O)	6.34	0.56	0.56
	assign (segid 3A4 and resid 35 and name O)	(segid 3A4 and resid 349 and name C)	6.69	0.29	0.30
	assign (segid 3A4 and resid 35 and name O)	(segid 3A4 and resid 349 and name O)	6.60	0.42	0.42
	assign (segid 3A4 and resid 35 and name O)	(segid 3A4 and resid 350 and name C)	5.39	0.37	0.37
40	assign (segid 3A4 and resid 35 and name O)	(segid 3A4 and resid 350 and name CB)	5.15	0.56	0.56
	assign (segid 3A4 and resid 35 and name O)	(segid 3A4 and resid 350 and name N)	5.91	0.28	0.27
	assign (segid 3A4 and resid 35 and name O)	(segid 3A4 and resid 36 and name C)	2.92	0.05	0.06
	assign (segid 3A4 and resid 35 and name O)	(segid 3A4 and resid 36 and name CA)	2.76	0.04	0.04
	assign (segid 3A4 and resid 35 and name O)	(segid 3A4 and resid 36 and name N)	2.25	0.03	0.02
45	assign (segid 3A4 and resid 35 and name O)	(segid 3A4 and resid 36 and name O)	3.43	0.12	0.11
	assign (segid 3A4 and resid 35 and name O)	(segid 3A4 and resid 37 and name C)	4.08	0.17	0.17
	assign (segid 3A4 and resid 35 and name O)	(segid 3A4 and resid 37 and name CA)	4.30	0.16	0.16
	assign (segid 3A4 and resid 35 and name O)	(segid 3A4 and resid 37 and name CB)	5.16	0.24	0.24
	assign (segid 3A4 and resid 35 and name O)	(segid 3A4 and resid 37 and name N)	3.35	0.15	0.14
50	assign (segid 3A4 and resid 35 and name O)	(segid 3A4 and resid 37 and name O)	5.03	0.16	0.16
	assign (segid 3A4 and resid 35 and name O)	(segid 3A4 and resid 38 and name C)	3.87	0.13	0.14
	assign (segid 3A4 and resid 35 and name O)	(segid 3A4 and resid 38 and name CA)	3.82	0.16	0.16
	assign (segid 3A4 and resid 35 and name O)	(segid 3A4 and resid 38 and name CB)	3.83	0.15	0.16
	assign (segid 3A4 and resid 35 and name O)	(segid 3A4 and resid 38 and name N)	3.29	0.19	0.18
55	assign (segid 3A4 and resid 35 and name O)	(segid 3A4 and resid 38 and name O)	5.04	0.13	0.13
	assign (segid 3A4 and resid 35 and name O)	(segid 3A4 and resid 39 and name C)	4.98	0.14	0.13
	assign (segid 3A4 and resid 35 and name O)	(segid 3A4 and resid 39 and name CA)	3.86	0.14	0.14
	assign (segid 3A4 and resid 35 and name O)	(segid 3A4 and resid 39 and name CB)	3.52	0.19	0.19
60	assign (segid 3A4 and resid 35 and name O)	(segid 3A4 and resid 39 and name N)	3.01	0.13	0.12
	assign (segid 3A4 and resid 35 and name O)	(segid 3A4 and resid 40 and name C)	7.22	0.13	0.13
	assign (segid 3A4 and resid 35 and name O)	(segid 3A4 and resid 40 and name CA)	6.39	0.14	0.13
	assign (segid 3A4 and resid 35 and name O)	(segid 3A4 and resid 40 and name CB)	6.67	0.14	0.14
	assign (segid 3A4 and resid 35 and name O)	(segid 3A4 and resid 40 and name N)	5.02	0.14	0.14
65	assign (segid 3A4 and resid 35 and name O)	(segid 3A4 and resid 41 and name CB)	7.68	0.15	0.16
	assign (segid 3A4 and resid 35 and name O)	(segid 3A4 and resid 41 and name N)	6.84	0.15	0.16
	assign (segid 3A4 and resid 35 and name O)	(segid 3A4 and resid 360 and name CB)	2.55	0.04	0.04
	assign (segid 3A4 and resid 360 and name C)	(segid 3A4 and resid 360 and name O)	1.23	0.00	0.00
70	assign (segid 3A4 and resid 360 and name C)	(segid 3A4 and resid 361 and name C)	3.22	0.02	0.03
	assign (segid 3A4 and resid 360 and name C)	(segid 3A4 and resid 361 and name CA)	2.42	0.02	0.01
	assign (segid 3A4 and resid 360 and name C)	(segid 3A4 and resid 361 and name CB)	3.62	0.04	0.04
	assign (segid 3A4 and resid 360 and name C)	(segid 3A4 and resid 361 and name N)	1.33	0.01	0.00
	assign (segid 3A4 and resid 360 and name C)	(segid 3A4 and resid 361 and name O)	4.33	0.06	0.05
75	assign (segid 3A4 and resid 360 and name C)	(segid 3A4 and resid 362 and name C)	4.88	0.08	0.09
	assign (segid 3A4 and resid 360 and name C)	(segid 3A4 and resid 362 and name CA)	4.55	0.08	0.07
	assign (segid 3A4 and resid 360 and name C)	(segid 3A4 and resid 362 and name CB)	5.23	0.10	0.10
	assign (segid 3A4 and resid 360 and name C)	(segid 3A4 and resid 362 and name N)	3.22	0.08	0.08
	assign (segid 3A4 and resid 360 and name C)	(segid 3A4 and resid 362 and name O)	4.46	0.11	0.11
80	assign (segid 3A4 and resid 360 and name C)	(segid 3A4 and resid 363 and name C)	7.68	0.07	0.06
	assign (segid 3A4 and resid 360 and name C)	(segid 3A4 and resid 363 and name CA)	6.85	0.14	0.14
	assign (segid 3A4 and resid 360 and name C)	(segid 3A4 and resid 363 and name N)	6.04	0.14	0.14
	assign (segid 3A4 and resid 360 and name C)	(segid 3A4 and resid 364 and name N)	7.70	0.05	0.06

	assign (segid 3A4 and resid 360 and name CA)	(segid 3A4 and resid 360 and name C)	1.51	0.02	0.02
	assign (segid 3A4 and resid 360 and name CA)	(segid 3A4 and resid 360 and name CB)	1.54	0.03	0.02
	assign (segid 3A4 and resid 360 and name CA)	(segid 3A4 and resid 360 and name O)	2.39	0.02	0.01
	assign (segid 3A4 and resid 360 and name CA)	(segid 3A4 and resid 361 and name C)	4.54	0.03	0.03
5	assign (segid 3A4 and resid 360 and name CA)	(segid 3A4 and resid 361 and name CA)	3.78	0.01	0.01
	assign (segid 3A4 and resid 360 and name CA)	(segid 3A4 and resid 361 and name CB)	4.78	0.06	0.06
	assign (segid 3A4 and resid 360 and name CA)	(segid 3A4 and resid 361 and name N)	2.42	0.02	0.03
	assign (segid 3A4 and resid 360 and name CA)	(segid 3A4 and resid 361 and name O)	5.71	0.06	0.05
	assign (segid 3A4 and resid 360 and name CA)	(segid 3A4 and resid 362 and name C)	5.78	0.09	0.09
	assign (segid 3A4 and resid 360 and name CA)	(segid 3A4 and resid 362 and name CA)	5.47	0.06	0.07
10	assign (segid 3A4 and resid 360 and name CA)	(segid 3A4 and resid 362 and name CB)	5.81	0.09	0.10
	assign (segid 3A4 and resid 360 and name CA)	(segid 3A4 and resid 362 and name N)	4.26	0.06	0.06
	assign (segid 3A4 and resid 360 and name CA)	(segid 3A4 and resid 362 and name O)	5.17	0.10	0.09
	assign (segid 3A4 and resid 360 and name CA)	(segid 3A4 and resid 363 and name CA)	7.77	0.13	0.13
	assign (segid 3A4 and resid 360 and name CA)	(segid 3A4 and resid 363 and name CB)	8.98	0.19	0.18
15	assign (segid 3A4 and resid 360 and name CA)	(segid 3A4 and resid 363 and name N)	7.03	0.12	0.11
	assign (segid 3A4 and resid 360 and name CA)	(segid 3A4 and resid 364 and name CA)	9.11	0.13	0.12
	assign (segid 3A4 and resid 360 and name CA)	(segid 3A4 and resid 364 and name CB)	8.53	0.16	0.17
	assign (segid 3A4 and resid 360 and name CA)	(segid 3A4 and resid 365 and name CA)	11.89	0.30	0.30
	assign (segid 3A4 and resid 360 and name CA)	(segid 3A4 and resid 365 and name CB)	13.22	0.25	0.26
20	assign (segid 3A4 and resid 360 and name CA)	(segid 3A4 and resid 365 and name N)	11.40	0.63	0.63
	assign (segid 3A4 and resid 360 and name CA)	(segid 3A4 and resid 381 and name CA)	13.86	0.66	0.66
	assign (segid 3A4 and resid 360 and name CA)	(segid 3A4 and resid 382 and name CA)	14.07	0.79	0.78
	assign (segid 3A4 and resid 360 and name CA)	(segid 3A4 and resid 382 and name CB)	14.27	0.60	0.60
	assign (segid 3A4 and resid 360 and name CA)	(segid 3A4 and resid 383 and name CA)	17.92	0.62	0.61
25	assign (segid 3A4 and resid 360 and name CA)	(segid 3A4 and resid 384 and name CA)	18.03	0.79	0.80
	assign (segid 3A4 and resid 360 and name CA)	(segid 3A4 and resid 433 and name CA)	18.97	0.87	0.88
	assign (segid 3A4 and resid 360 and name CA)	(segid 3A4 and resid 434 and name CA)	5.66	0.04	0.05
	assign (segid 3A4 and resid 360 and name CB)	(segid 3A4 and resid 361 and name C)	4.59	0.07	0.07
	assign (segid 3A4 and resid 360 and name CB)	(segid 3A4 and resid 361 and name CB)	5.32	0.13	0.13
30	assign (segid 3A4 and resid 360 and name CB)	(segid 3A4 and resid 361 and name N)	3.30	0.07	0.06
	assign (segid 3A4 and resid 360 and name CB)	(segid 3A4 and resid 361 and name O)	6.78	0.03	0.02
	assign (segid 3A4 and resid 360 and name CB)	(segid 3A4 and resid 362 and name C)	7.24	0.11	0.11
	assign (segid 3A4 and resid 360 and name CB)	(segid 3A4 and resid 362 and name CA)	6.91	0.08	0.08
	assign (segid 3A4 and resid 360 and name CB)	(segid 3A4 and resid 362 and name CB)	7.29	0.10	0.10
35	assign (segid 3A4 and resid 360 and name CB)	(segid 3A4 and resid 362 and name N)	5.61	0.08	0.09
	assign (segid 3A4 and resid 360 and name CB)	(segid 3A4 and resid 362 and name O)	6.62	0.12	0.12
	assign (segid 3A4 and resid 360 and name CB)	(segid 3A4 and resid 363 and name CA)	9.16	0.18	0.17
	assign (segid 3A4 and resid 360 and name CB)	(segid 3A4 and resid 363 and name CB)	10.30	0.24	0.24
40	assign (segid 3A4 and resid 360 and name CB)	(segid 3A4 and resid 364 and name CA)	10.54	0.11	0.12
	assign (segid 3A4 and resid 360 and name CB)	(segid 3A4 and resid 364 and name CB)	9.99	0.17	0.16
	assign (segid 3A4 and resid 360 and name CB)	(segid 3A4 and resid 365 and name CA)	13.17	0.29	0.29
	assign (segid 3A4 and resid 360 and name CB)	(segid 3A4 and resid 365 and name CB)	14.51	0.23	0.24
	assign (segid 3A4 and resid 360 and name CB)	(segid 3A4 and resid 381 and name CA)	11.07	0.73	0.72
45	assign (segid 3A4 and resid 360 and name CB)	(segid 3A4 and resid 382 and name CA)	13.30	0.78	0.78
	assign (segid 3A4 and resid 360 and name CB)	(segid 3A4 and resid 382 and name CB)	13.35	0.89	0.89
	assign (segid 3A4 and resid 360 and name CB)	(segid 3A4 and resid 383 and name CA)	13.95	0.71	0.71
	assign (segid 3A4 and resid 360 and name CB)	(segid 3A4 and resid 384 and name CA)	17.59	0.73	0.74
	assign (segid 3A4 and resid 360 and name CB)	(segid 3A4 and resid 433 and name CA)	17.89	0.84	0.83
50	assign (segid 3A4 and resid 360 and name N)	(segid 3A4 and resid 360 and name C)	2.51	0.03	0.02
	assign (segid 3A4 and resid 360 and name N)	(segid 3A4 and resid 360 and name CA)	1.46	0.01	0.01
	assign (segid 3A4 and resid 360 and name N)	(segid 3A4 and resid 360 and name CB)	2.35	0.04	0.04
	assign (segid 3A4 and resid 360 and name N)	(segid 3A4 and resid 360 and name O)	3.60	0.01	0.02
	assign (segid 3A4 and resid 360 and name N)	(segid 3A4 and resid 361 and name C)	4.83	0.06	0.07
55	assign (segid 3A4 and resid 360 and name N)	(segid 3A4 and resid 361 and name CA)	4.22	0.05	0.04
	assign (segid 3A4 and resid 360 and name N)	(segid 3A4 and resid 361 and name CB)	4.98	0.07	0.08
	assign (segid 3A4 and resid 360 and name N)	(segid 3A4 and resid 361 and name N)	2.80	0.04	0.04
	assign (segid 3A4 and resid 360 and name N)	(segid 3A4 and resid 361 and name O)	6.04	0.07	0.07
	assign (segid 3A4 and resid 360 and name N)	(segid 3A4 and resid 362 and name C)	6.05	0.08	0.07
60	assign (segid 3A4 and resid 360 and name N)	(segid 3A4 and resid 362 and name CA)	5.48	0.08	0.08
	assign (segid 3A4 and resid 360 and name N)	(segid 3A4 and resid 362 and name CB)	5.46	0.12	0.13
	assign (segid 3A4 and resid 360 and name N)	(segid 3A4 and resid 362 and name N)	4.37	0.08	0.07
	assign (segid 3A4 and resid 360 and name N)	(segid 3A4 and resid 362 and name O)	5.55	0.09	0.09
	assign (segid 3A4 and resid 360 and name N)	(segid 3A4 and resid 363 and name N)	7.35	0.07	0.08
65	assign (segid 3A4 and resid 360 and name O)	(segid 3A4 and resid 360 and name CB)	3.26	0.05	0.05
	assign (segid 3A4 and resid 360 and name O)	(segid 3A4 and resid 361 and name C)	3.34	0.03	0.02
	assign (segid 3A4 and resid 360 and name O)	(segid 3A4 and resid 361 and name CA)	2.73	0.03	0.04
	assign (segid 3A4 and resid 360 and name O)	(segid 3A4 and resid 361 and name CB)	4.11	0.05	0.04
	assign (segid 3A4 and resid 360 and name O)	(segid 3A4 and resid 361 and name N)	2.23	0.01	0.02
70	assign (segid 3A4 and resid 360 and name O)	(segid 3A4 and resid 361 and name O)	4.25	0.10	0.09
	assign (segid 3A4 and resid 360 and name O)	(segid 3A4 and resid 362 and name C)	4.61	0.14	0.13
	assign (segid 3A4 and resid 360 and name O)	(segid 3A4 and resid 362 and name CA)	4.61	0.10	0.11
	assign (segid 3A4 and resid 360 and name O)	(segid 3A4 and resid 362 and name CB)	5.54	0.13	0.13
	assign (segid 3A4 and resid 360 and name O)	(segid 3A4 and resid 362 and name N)	3.44	0.12	0.11
75	assign (segid 3A4 and resid 360 and name O)	(segid 3A4 and resid 362 and name O)	4.10	0.17	0.16
	assign (segid 3A4 and resid 360 and name O)	(segid 3A4 and resid 363 and name C)	7.20	0.12	0.12
	assign (segid 3A4 and resid 360 and name O)	(segid 3A4 and resid 363 and name CA)	6.25	0.20	0.20
	assign (segid 3A4 and resid 360 and name O)	(segid 3A4 and resid 363 and name CB)	7.23	0.27	0.27
	assign (segid 3A4 and resid 360 and name O)	(segid 3A4 and resid 363 and name N)	5.63	0.19	0.19
80	assign (segid 3A4 and resid 360 and name O)	(segid 3A4 and resid 364 and name N)	7.21	0.04	0.05
	assign (segid 3A4 and resid 361 and name C)	(segid 3A4 and resid 361 and name CB)	2.50	0.03	0.03
	assign (segid 3A4 and resid 361 and name C)	(segid 3A4 and resid 361 and name O)	1.23	0.01	0.00
	assign (segid 3A4 and resid 361 and name C)	(segid 3A4 and resid 362 and name C)	3.30	0.07	0.08

	assign (segid 3A4 and resid 361 and name C) (segid 3A4 and resid 362 and name CA)	2.42	0.00	0.01
	assign (segid 3A4 and resid 361 and name C) (segid 3A4 and resid 362 and name CB)	3.60	0.04	0.04
	assign (segid 3A4 and resid 361 and name C) (segid 3A4 and resid 362 and name N)	1.32	0.02	0.01
	assign (segid 3A4 and resid 361 and name C) (segid 3A4 and resid 362 and name O)	3.78	0.13	0.12
	assign (segid 3A4 and resid 361 and name C) (segid 3A4 and resid 363 and name C)	6.33	0.07	0.08
5	assign (segid 3A4 and resid 361 and name C) (segid 3A4 and resid 363 and name CA)	5.33	0.08	0.09
	assign (segid 3A4 and resid 361 and name C) (segid 3A4 and resid 363 and name CB)	6.09	0.13	0.14
	assign (segid 3A4 and resid 361 and name C) (segid 3A4 and resid 363 and name CG)	7.43	0.10	0.10
	assign (segid 3A4 and resid 361 and name C) (segid 3A4 and resid 363 and name N)	4.12	0.10	0.09
	assign (segid 3A4 and resid 361 and name C) (segid 3A4 and resid 363 and name O)	6.89	0.12	0.12
10	assign (segid 3A4 and resid 361 and name C) (segid 3A4 and resid 364 and name N)	6.89	0.10	0.10
	assign (segid 3A4 and resid 361 and name C) (segid 3A4 and resid 361 and name C)	1.53	0.02	0.01
	assign (segid 3A4 and resid 361 and name CA) (segid 3A4 and resid 361 and name C)	1.51	0.02	0.02
	assign (segid 3A4 and resid 361 and name CA) (segid 3A4 and resid 361 and name CB)	2.38	0.02	0.02
	assign (segid 3A4 and resid 361 and name CA) (segid 3A4 and resid 362 and name C)	4.59	0.06	0.07
15	assign (segid 3A4 and resid 361 and name CA) (segid 3A4 and resid 362 and name CA)	3.82	0.02	0.02
	assign (segid 3A4 and resid 361 and name CA) (segid 3A4 and resid 362 and name CB)	4.81	0.06	0.07
	assign (segid 3A4 and resid 361 and name CA) (segid 3A4 and resid 362 and name N)	2.45	0.03	0.03
	assign (segid 3A4 and resid 361 and name CA) (segid 3A4 and resid 362 and name O)	4.79	0.12	0.11
	assign (segid 3A4 and resid 361 and name CA) (segid 3A4 and resid 363 and name C)	7.63	0.07	0.07
20	assign (segid 3A4 and resid 361 and name CA) (segid 3A4 and resid 363 and name CA)	6.59	0.09	0.10
	assign (segid 3A4 and resid 361 and name CA) (segid 3A4 and resid 363 and name CB)	7.36	0.16	0.16
	assign (segid 3A4 and resid 361 and name CA) (segid 3A4 and resid 363 and name N)	5.50	0.11	0.11
	assign (segid 3A4 and resid 361 and name CA) (segid 3A4 and resid 364 and name CA)	9.24	0.09	0.08
	assign (segid 3A4 and resid 361 and name CA) (segid 3A4 and resid 364 and name CB)	9.00	0.14	0.14
25	assign (segid 3A4 and resid 361 and name CA) (segid 3A4 and resid 365 and name CA)	12.40	0.14	0.14
	assign (segid 3A4 and resid 361 and name CA) (segid 3A4 and resid 365 and name CB)	13.46	0.12	0.12
	assign (segid 3A4 and resid 361 and name CA) (segid 3A4 and resid 381 and name CA)	13.82	0.60	0.59
	assign (segid 3A4 and resid 361 and name CA) (segid 3A4 and resid 382 and name CA)	15.83	0.54	0.54
	assign (segid 3A4 and resid 361 and name CA) (segid 3A4 and resid 382 and name CB)	16.11	0.67	0.66
30	assign (segid 3A4 and resid 361 and name CA) (segid 3A4 and resid 383 and name CA)	15.42	0.51	0.50
	assign (segid 3A4 and resid 361 and name CA) (segid 3A4 and resid 426 and name CA)	16.59	1.66	1.66
	assign (segid 3A4 and resid 361 and name CA) (segid 3A4 and resid 433 and name CA)	16.47	0.85	0.84
	assign (segid 3A4 and resid 361 and name CA) (segid 3A4 and resid 434 and name CA)	17.02	0.86	0.86
	assign (segid 3A4 and resid 361 and name CA) (segid 3A4 and resid 435 and name CA)	17.50	1.18	1.18
35	assign (segid 3A4 and resid 361 and name CB) (segid 3A4 and resid 362 and name C)	5.79	0.09	0.09
	assign (segid 3A4 and resid 361 and name CB) (segid 3A4 and resid 362 and name CB)	4.77	0.05	0.06
	assign (segid 3A4 and resid 361 and name CB) (segid 3A4 and resid 362 and name CB)	5.63	0.03	0.03
	assign (segid 3A4 and resid 361 and name CB) (segid 3A4 and resid 362 and name N)	3.53	0.05	0.05
	assign (segid 3A4 and resid 361 and name CB) (segid 3A4 and resid 362 and name O)	6.14	0.12	0.12
40	assign (segid 3A4 and resid 361 and name CB) (segid 3A4 and resid 363 and name CA)	7.79	0.11	0.11
	assign (segid 3A4 and resid 361 and name CB) (segid 3A4 and resid 363 and name CB)	8.44	0.17	0.17
	assign (segid 3A4 and resid 361 and name CB) (segid 3A4 and resid 363 and name N)	6.59	0.11	0.12
	assign (segid 3A4 and resid 361 and name CB) (segid 3A4 and resid 364 and name CA)	10.52	0.12	0.11
	assign (segid 3A4 and resid 361 and name CB) (segid 3A4 and resid 364 and name CB)	10.24	0.17	0.18
45	assign (segid 3A4 and resid 361 and name CB) (segid 3A4 and resid 365 and name CA)	13.78	0.14	0.14
	assign (segid 3A4 and resid 361 and name CB) (segid 3A4 and resid 365 and name CB)	14.80	0.13	0.14
	assign (segid 3A4 and resid 361 and name CB) (segid 3A4 and resid 381 and name CA)	15.03	0.60	0.60
	assign (segid 3A4 and resid 361 and name CB) (segid 3A4 and resid 382 and name CA)	16.88	0.55	0.56
	assign (segid 3A4 and resid 361 and name CB) (segid 3A4 and resid 382 and name CB)	17.06	0.68	0.68
50	assign (segid 3A4 and resid 361 and name CB) (segid 3A4 and resid 383 and name CA)	16.47	0.53	0.53
	assign (segid 3A4 and resid 361 and name CB) (segid 3A4 and resid 424 and name CA)	16.95	2.09	2.09
	assign (segid 3A4 and resid 361 and name CB) (segid 3A4 and resid 426 and name CA)	16.42	1.59	1.60
	assign (segid 3A4 and resid 361 and name CB) (segid 3A4 and resid 427 and name CA)	17.64	1.64	1.63
	assign (segid 3A4 and resid 361 and name CB) (segid 3A4 and resid 433 and name CA)	16.73	0.88	0.89
55	assign (segid 3A4 and resid 361 and name CB) (segid 3A4 and resid 434 and name CA)	17.33	0.84	0.85
	assign (segid 3A4 and resid 361 and name CB) (segid 3A4 and resid 435 and name CA)	17.72	1.16	1.17
	assign (segid 3A4 and resid 361 and name CB) (segid 3A4 and resid 361 and name C)	2.47	0.02	0.02
	assign (segid 3A4 and resid 361 and name N) (segid 3A4 and resid 361 and name CA)	1.45	0.01	0.00
	assign (segid 3A4 and resid 361 and name N) (segid 3A4 and resid 361 and name CB)	2.43	0.04	0.03
60	assign (segid 3A4 and resid 361 and name N) (segid 3A4 and resid 361 and name O)	3.59	0.02	0.03
	assign (segid 3A4 and resid 361 and name N) (segid 3A4 and resid 362 and name C)	4.89	0.06	0.05
	assign (segid 3A4 and resid 361 and name N) (segid 3A4 and resid 362 and name CA)	4.17	0.04	0.04
	assign (segid 3A4 and resid 361 and name N) (segid 3A4 and resid 362 and name CB)	4.84	0.09	0.10
	assign (segid 3A4 and resid 361 and name N) (segid 3A4 and resid 362 and name N)	2.72	0.04	0.05
65	assign (segid 3A4 and resid 361 and name N) (segid 3A4 and resid 362 and name O)	4.78	0.09	0.09
	assign (segid 3A4 and resid 361 and name N) (segid 3A4 and resid 363 and name C)	7.90	0.03	0.03
	assign (segid 3A4 and resid 361 and name N) (segid 3A4 and resid 363 and name CA)	7.04	0.09	0.09
	assign (segid 3A4 and resid 361 and name N) (segid 3A4 and resid 363 and name N)	6.01	0.09	0.09
	assign (segid 3A4 and resid 361 and name N) (segid 3A4 and resid 361 and name CB)	2.95	0.05	0.05
70	assign (segid 3A4 and resid 361 and name O) (segid 3A4 and resid 362 and name C)	3.50	0.16	0.16
	assign (segid 3A4 and resid 361 and name O) (segid 3A4 and resid 362 and name CA)	2.74	0.04	0.03
	assign (segid 3A4 and resid 361 and name O) (segid 3A4 and resid 362 and name CB)	4.06	0.06	0.06
	assign (segid 3A4 and resid 361 and name O) (segid 3A4 and resid 362 and name N)	2.22	0.02	0.02
	assign (segid 3A4 and resid 361 and name O) (segid 3A4 and resid 362 and name O)	4.23	0.21	0.22
75	assign (segid 3A4 and resid 361 and name O) (segid 3A4 and resid 363 and name C)	6.28	0.16	0.15
	assign (segid 3A4 and resid 361 and name O) (segid 3A4 and resid 363 and name CA)	5.15	0.18	0.18
	assign (segid 3A4 and resid 361 and name O) (segid 3A4 and resid 363 and name CB)	5.64	0.22	0.21
	assign (segid 3A4 and resid 361 and name O) (segid 3A4 and resid 363 and name CG)	7.01	0.20	0.21
	assign (segid 3A4 and resid 361 and name O) (segid 3A4 and resid 363 and name N)	3.94	0.15	0.15
80	assign (segid 3A4 and resid 361 and name O) (segid 3A4 and resid 363 and name O)	6.73	0.16	0.15
	assign (segid 3A4 and resid 361 and name O) (segid 3A4 and resid 364 and name N)	7.03	0.17	0.16
	assign (segid 3A4 and resid 362 and name C) (segid 3A4 and resid 362 and name CB)	2.49	0.04	0.04

	assign (segid 3A4 and resid 362 and name C) (segid 3A4 and resid 362 and name O)	1.24	0.01	0.00
	assign (segid 3A4 and resid 362 and name C) (segid 3A4 and resid 363 and name C)	3.10	0.05	0.05
	assign (segid 3A4 and resid 362 and name C) (segid 3A4 and resid 363 and name CA)	2.43	0.01	0.01
	assign (segid 3A4 and resid 362 and name C) (segid 3A4 and resid 363 and name CB)	3.68	0.02	0.02
	assign (segid 3A4 and resid 362 and name C) (segid 3A4 and resid 363 and name CG)	4.92	0.02	0.02
5	assign (segid 3A4 and resid 362 and name C) (segid 3A4 and resid 363 and name N)	1.33	0.00	0.01
	assign (segid 3A4 and resid 362 and name C) (segid 3A4 and resid 363 and name O)	3.76	0.10	0.10
	assign (segid 3A4 and resid 362 and name C) (segid 3A4 and resid 364 and name C)	5.98	0.11	0.11
	assign (segid 3A4 and resid 362 and name C) (segid 3A4 and resid 364 and name CA)	4.81	0.09	0.09
	assign (segid 3A4 and resid 362 and name C) (segid 3A4 and resid 364 and name CB)	4.81	0.13	0.13
10	assign (segid 3A4 and resid 362 and name C) (segid 3A4 and resid 364 and name N)	3.64	0.08	0.08
	assign (segid 3A4 and resid 362 and name C) (segid 3A4 and resid 364 and name O)	6.26	0.18	0.19
	assign (segid 3A4 and resid 362 and name C) (segid 3A4 and resid 365 and name N)	6.95	0.08	0.09
	assign (segid 3A4 and resid 362 and name C) (segid 3A4 and resid 362 and name C)	1.53	0.01	0.00
	assign (segid 3A4 and resid 362 and name CA) (segid 3A4 and resid 362 and name CB)	1.53	0.01	0.01
15	assign (segid 3A4 and resid 362 and name CA) (segid 3A4 and resid 362 and name O)	2.41	0.01	0.01
	assign (segid 3A4 and resid 362 and name CA) (segid 3A4 and resid 363 and name C)	4.40	0.05	0.05
	assign (segid 3A4 and resid 362 and name CA) (segid 3A4 and resid 363 and name CA)	3.81	0.01	0.01
	assign (segid 3A4 and resid 362 and name CA) (segid 3A4 and resid 363 and name CB)	4.85	0.03	0.04
	assign (segid 3A4 and resid 362 and name CA) (segid 3A4 and resid 363 and name CG)	6.23	0.03	0.03
20	assign (segid 3A4 and resid 362 and name CA) (segid 3A4 and resid 363 and name N)	2.44	0.01	0.02
	assign (segid 3A4 and resid 362 and name CA) (segid 3A4 and resid 363 and name O)	4.79	0.12	0.11
	assign (segid 3A4 and resid 362 and name CA) (segid 3A4 and resid 364 and name C)	7.27	0.11	0.11
	assign (segid 3A4 and resid 362 and name CA) (segid 3A4 and resid 364 and name CA)	6.00	0.08	0.09
	assign (segid 3A4 and resid 362 and name CA) (segid 3A4 and resid 364 and name CB)	5.74	0.15	0.16
25	assign (segid 3A4 and resid 362 and name CA) (segid 3A4 and resid 364 and name N)	4.99	0.08	0.08
	assign (segid 3A4 and resid 362 and name CA) (segid 3A4 and resid 364 and name O)	7.55	0.19	0.19
	assign (segid 3A4 and resid 362 and name CA) (segid 3A4 and resid 365 and name CA)	9.56	0.10	0.10
	assign (segid 3A4 and resid 362 and name CA) (segid 3A4 and resid 365 and name CB)	10.53	0.08	0.09
	assign (segid 3A4 and resid 362 and name CA) (segid 3A4 and resid 381 and name CA)	14.74	0.56	0.55
30	assign (segid 3A4 and resid 362 and name CA) (segid 3A4 and resid 382 and name CA)	17.29	0.50	0.49
	assign (segid 3A4 and resid 362 and name CA) (segid 3A4 and resid 382 and name CB)	17.84	0.63	0.63
	assign (segid 3A4 and resid 362 and name CA) (segid 3A4 and resid 383 and name CA)	16.69	0.44	0.45
	assign (segid 3A4 and resid 362 and name CA) (segid 3A4 and resid 405 and name CB)	18.70	0.43	0.44
	assign (segid 3A4 and resid 362 and name CA) (segid 3A4 and resid 433 and name CA)	18.32	0.92	0.93
35	assign (segid 3A4 and resid 362 and name CA) (segid 3A4 and resid 434 and name CA)	18.29	0.93	0.92
	assign (segid 3A4 and resid 362 and name CA) (segid 3A4 and resid 435 and name CA)	18.29	1.30	1.30
	assign (segid 3A4 and resid 362 and name CB) (segid 3A4 and resid 363 and name C)	4.73	0.14	0.13
	assign (segid 3A4 and resid 362 and name CB) (segid 3A4 and resid 363 and name CA)	4.61	0.08	0.08
	assign (segid 3A4 and resid 362 and name CB) (segid 3A4 and resid 363 and name CB)	5.77	0.12	0.13
40	assign (segid 3A4 and resid 362 and name CB) (segid 3A4 and resid 363 and name CG)	7.08	0.11	0.11
	assign (segid 3A4 and resid 362 and name CB) (segid 3A4 and resid 363 and name N)	3.36	0.08	0.08
	assign (segid 3A4 and resid 362 and name CB) (segid 3A4 and resid 363 and name O)	4.91	0.20	0.20
	assign (segid 3A4 and resid 362 and name CB) (segid 3A4 and resid 364 and name C)	7.20	0.20	0.19
	assign (segid 3A4 and resid 362 and name CB) (segid 3A4 and resid 364 and name CA)	5.85	0.18	0.18
45	assign (segid 3A4 and resid 362 and name CB) (segid 3A4 and resid 364 and name CB)	5.25	0.24	0.23
	assign (segid 3A4 and resid 362 and name CB) (segid 3A4 and resid 364 and name N)	5.16	0.16	0.16
	assign (segid 3A4 and resid 362 and name CB) (segid 3A4 and resid 364 and name O)	7.47	0.25	0.25
	assign (segid 3A4 and resid 362 and name CB) (segid 3A4 and resid 365 and name CA)	9.58	0.19	0.19
	assign (segid 3A4 and resid 362 and name CB) (segid 3A4 and resid 365 and name CB)	10.60	0.17	0.16
50	assign (segid 3A4 and resid 362 and name CB) (segid 3A4 and resid 381 and name CA)	15.37	0.59	0.60
	assign (segid 3A4 and resid 362 and name CB) (segid 3A4 and resid 382 and name CA)	18.13	0.55	0.54
	assign (segid 3A4 and resid 362 and name CB) (segid 3A4 and resid 383 and name CA)	17.74	0.49	0.49
	assign (segid 3A4 and resid 362 and name N) (segid 3A4 and resid 362 and name C)	2.45	0.03	0.03
	assign (segid 3A4 and resid 362 and name N) (segid 3A4 and resid 362 and name CA)	1.46	0.01	0.01
55	assign (segid 3A4 and resid 362 and name N) (segid 3A4 and resid 362 and name CB)	2.46	0.02	0.01
	assign (segid 3A4 and resid 362 and name N) (segid 3A4 and resid 362 and name O)	2.85	0.06	0.06
	assign (segid 3A4 and resid 362 and name N) (segid 3A4 and resid 363 and name C)	5.54	0.04	0.04
	assign (segid 3A4 and resid 362 and name N) (segid 3A4 and resid 363 and name CA)	4.77	0.04	0.05
	assign (segid 3A4 and resid 362 and name N) (segid 3A4 and resid 363 and name CB)	5.79	0.07	0.08
60	assign (segid 3A4 and resid 362 and name N) (segid 3A4 and resid 363 and name CG)	7.12	0.06	0.06
	assign (segid 3A4 and resid 362 and name N) (segid 3A4 and resid 363 and name N)	3.53	0.06	0.06
	assign (segid 3A4 and resid 362 and name N) (segid 3A4 and resid 363 and name O)	6.09	0.10	0.11
	assign (segid 3A4 and resid 362 and name N) (segid 3A4 and resid 364 and name CA)	7.05	0.11	0.12
	assign (segid 3A4 and resid 362 and name N) (segid 3A4 and resid 364 and name CB)	6.73	0.16	0.16
65	assign (segid 3A4 and resid 362 and name N) (segid 3A4 and resid 364 and name N)	5.98	0.11	0.11
	assign (segid 3A4 and resid 362 and name N) (segid 3A4 and resid 362 and name CB)	3.08	0.06	0.07
	assign (segid 3A4 and resid 362 and name O) (segid 3A4 and resid 363 and name C)	3.26	0.09	0.09
	assign (segid 3A4 and resid 362 and name O) (segid 3A4 and resid 363 and name CA)	2.75	0.02	0.02
	assign (segid 3A4 and resid 362 and name O) (segid 3A4 and resid 363 and name CB)	4.17	0.04	0.03
70	assign (segid 3A4 and resid 362 and name O) (segid 3A4 and resid 363 and name CG)	5.15	0.05	0.05
	assign (segid 3A4 and resid 362 and name O) (segid 3A4 and resid 363 and name N)	2.24	0.02	0.02
	assign (segid 3A4 and resid 362 and name O) (segid 3A4 and resid 363 and name O)	4.18	0.12	0.11
	assign (segid 3A4 and resid 362 and name O) (segid 3A4 and resid 364 and name C)	5.46	0.17	0.18
	assign (segid 3A4 and resid 362 and name O) (segid 3A4 and resid 364 and name CA)	4.50	0.15	0.15
75	assign (segid 3A4 and resid 362 and name O) (segid 3A4 and resid 364 and name CB)	4.43	0.18	0.17
	assign (segid 3A4 and resid 362 and name O) (segid 3A4 and resid 364 and name N)	3.34	0.14	0.14
	assign (segid 3A4 and resid 362 and name O) (segid 3A4 and resid 364 and name O)	5.54	0.25	0.24
	assign (segid 3A4 and resid 362 and name O) (segid 3A4 and resid 365 and name N)	6.56	0.16	0.16
	assign (segid 3A4 and resid 362 and name O) (segid 3A4 and resid 363 and name CB)	2.50	0.04	0.05
80	assign (segid 3A4 and resid 363 and name C) (segid 3A4 and resid 363 and name O)	3.05	0.02	0.02
	assign (segid 3A4 and resid 363 and name C) (segid 3A4 and resid 363 and name O)	1.23	0.01	0.01
	assign (segid 3A4 and resid 363 and name C) (segid 3A4 and resid 364 and name C)	3.57	0.04	0.04

	assign (segid 3A4 and resid 363 and name C) (segid 3A4 and resid 364 and name CA)	2.12	0.02	0.02
	assign (segid 3A4 and resid 363 and name C) (segid 3A4 and resid 364 and name CB)	3.28	0.08	0.09
	assign (segid 3A4 and resid 363 and name C) (segid 3A4 and resid 364 and name N)	1.32	0.00	0.01
	assign (segid 3A4 and resid 363 and name C) (segid 3A4 and resid 364 and name O)	1.33	0.05	0.05
	assign (segid 3A4 and resid 363 and name C) (segid 3A4 and resid 365 and name C)	6.55	0.05	0.05
5	assign (segid 3A4 and resid 363 and name C) (segid 3A4 and resid 365 and name CA)	5.54	0.10	0.09
	assign (segid 3A4 and resid 363 and name C) (segid 3A4 and resid 365 and name CB)	6.28	0.13	0.13
	assign (segid 3A4 and resid 363 and name C) (segid 3A4 and resid 365 and name N)	4.21	0.10	0.10
	assign (segid 3A4 and resid 363 and name C) (segid 3A4 and resid 365 and name O)	7.59	0.09	0.09
	assign (segid 3A4 and resid 363 and name C) (segid 3A4 and resid 365 and name C)	1.51	0.01	0.01
10	assign (segid 3A4 and resid 363 and name CA) (segid 3A4 and resid 363 and name CB)	1.53	0.02	0.02
	assign (segid 3A4 and resid 363 and name CA) (segid 3A4 and resid 363 and name CG)	2.54	0.02	0.01
	assign (segid 3A4 and resid 363 and name CA) (segid 3A4 and resid 363 and name O)	2.38	0.02	0.02
	assign (segid 3A4 and resid 363 and name CA) (segid 3A4 and resid 364 and name C)	4.77	0.03	0.03
	assign (segid 3A4 and resid 363 and name CA) (segid 3A4 and resid 364 and name CA)	3.80	0.01	0.01
15	assign (segid 3A4 and resid 363 and name CA) (segid 3A4 and resid 364 and name CB)	4.56	0.07	0.07
	assign (segid 3A4 and resid 363 and name CA) (segid 3A4 and resid 364 and name N)	2.44	0.03	0.02
	assign (segid 3A4 and resid 363 and name CA) (segid 3A4 and resid 364 and name O)	5.34	0.09	0.08
	assign (segid 3A4 and resid 363 and name CA) (segid 3A4 and resid 365 and name C)	7.69	0.06	0.06
	assign (segid 3A4 and resid 363 and name CA) (segid 3A4 and resid 365 and name CA)	6.60	0.08	0.08
20	assign (segid 3A4 and resid 363 and name CA) (segid 3A4 and resid 365 and name CB)	7.32	0.14	0.14
	assign (segid 3A4 and resid 363 and name CA) (segid 3A4 and resid 365 and name N)	5.41	0.09	0.09
	assign (segid 3A4 and resid 363 and name CA) (segid 3A4 and resid 381 and name CA)	13.86	0.57	0.56
	assign (segid 3A4 and resid 363 and name CA) (segid 3A4 and resid 382 and name CA)	16.39	0.48	0.48
	assign (segid 3A4 and resid 363 and name CA) (segid 3A4 and resid 382 and name CB)	17.23	0.60	0.60
25	assign (segid 3A4 and resid 363 and name CA) (segid 3A4 and resid 383 and name CA)	15.24	0.46	0.46
	assign (segid 3A4 and resid 363 and name CA) (segid 3A4 and resid 384 and name CA)	18.55	0.48	0.49
	assign (segid 3A4 and resid 363 and name CA) (segid 3A4 and resid 384 and name CB)	18.80	0.51	0.50
	assign (segid 3A4 and resid 363 and name CA) (segid 3A4 and resid 398 and name CA)	18.11	0.43	0.44
	assign (segid 3A4 and resid 363 and name CA) (segid 3A4 and resid 398 and name CB)	18.10	0.52	0.51
30	assign (segid 3A4 and resid 363 and name CA) (segid 3A4 and resid 401 and name CA)	16.95	0.40	0.40
	assign (segid 3A4 and resid 363 and name CA) (segid 3A4 and resid 402 and name CA)	17.18	0.34	0.34
	assign (segid 3A4 and resid 363 and name CA) (segid 3A4 and resid 402 and name CB)	17.67	0.31	0.31
	assign (segid 3A4 and resid 363 and name CA) (segid 3A4 and resid 405 and name CA)	16.28	0.44	0.44
	assign (segid 3A4 and resid 363 and name CA) (segid 3A4 and resid 405 and name CB)	14.95	0.44	0.44
35	assign (segid 3A4 and resid 363 and name CA) (segid 3A4 and resid 406 and name CA)	18.32	0.24	0.24
	assign (segid 3A4 and resid 363 and name CA) (segid 3A4 and resid 408 and name CB)	18.63	0.43	0.44
	assign (segid 3A4 and resid 363 and name CA) (segid 3A4 and resid 409 and name CA)	18.04	0.51	0.51
	assign (segid 3A4 and resid 363 and name CA) (segid 3A4 and resid 409 and name CB)	16.80	0.45	0.45
	assign (segid 3A4 and resid 363 and name CA) (segid 3A4 and resid 415 and name CA)	17.99	1.19	1.19
40	assign (segid 3A4 and resid 363 and name CA) (segid 3A4 and resid 433 and name CA)	17.21	0.96	0.95
	assign (segid 3A4 and resid 363 and name CA) (segid 3A4 and resid 434 and name CA)	16.73	1.04	1.03
	assign (segid 3A4 and resid 363 and name CA) (segid 3A4 and resid 435 and name CA)	16.60	1.27	1.28
	assign (segid 3A4 and resid 363 and name CB) (segid 3A4 and resid 363 and name CG)	1.51	0.01	0.01
	assign (segid 3A4 and resid 363 and name CB) (segid 3A4 and resid 364 and name C)	5.60	0.05	0.05
45	assign (segid 3A4 and resid 363 and name CB) (segid 3A4 and resid 364 and name CA)	4.77	0.05	0.06
	assign (segid 3A4 and resid 363 and name CB) (segid 3A4 and resid 364 and name CB)	5.77	0.11	0.11
	assign (segid 3A4 and resid 363 and name CB) (segid 3A4 and resid 364 and name N)	3.55	0.06	0.06
	assign (segid 3A4 and resid 363 and name CB) (segid 3A4 and resid 364 and name O)	6.31	0.10	0.10
	assign (segid 3A4 and resid 363 and name CB) (segid 3A4 and resid 365 and name CA)	7.04	0.12	0.12
50	assign (segid 3A4 and resid 363 and name CB) (segid 3A4 and resid 365 and name CB)	7.48	0.20	0.19
	assign (segid 3A4 and resid 363 and name CB) (segid 3A4 and resid 365 and name N)	5.94	0.10	0.11
	assign (segid 3A4 and resid 363 and name CB) (segid 3A4 and resid 381 and name CA)	14.58	0.62	0.62
	assign (segid 3A4 and resid 363 and name CB) (segid 3A4 and resid 382 and name CA)	16.90	0.51	0.51
	assign (segid 3A4 and resid 363 and name CB) (segid 3A4 and resid 382 and name CB)	17.78	0.61	0.61
55	assign (segid 3A4 and resid 363 and name CB) (segid 3A4 and resid 383 and name CA)	15.42	0.48	0.48
	assign (segid 3A4 and resid 363 and name CB) (segid 3A4 and resid 384 and name CA)	18.67	0.51	0.50
	assign (segid 3A4 and resid 363 and name CB) (segid 3A4 and resid 398 and name CA)	17.79	0.49	0.49
	assign (segid 3A4 and resid 363 and name CB) (segid 3A4 and resid 398 and name CB)	17.90	0.57	0.57
	assign (segid 3A4 and resid 363 and name CB) (segid 3A4 and resid 401 and name CA)	16.23	0.48	0.47
60	assign (segid 3A4 and resid 363 and name CB) (segid 3A4 and resid 402 and name CA)	16.60	0.43	0.43
	assign (segid 3A4 and resid 363 and name CB) (segid 3A4 and resid 402 and name CB)	17.20	0.41	0.41
	assign (segid 3A4 and resid 363 and name CB) (segid 3A4 and resid 404 and name CA)	18.42	0.70	0.69
	assign (segid 3A4 and resid 363 and name CB) (segid 3A4 and resid 404 and name CB)	18.00	0.83	0.83
	assign (segid 3A4 and resid 363 and name CB) (segid 3A4 and resid 405 and name CA)	15.33	0.50	0.50
65	assign (segid 3A4 and resid 363 and name CB) (segid 3A4 and resid 405 and name CB)	14.04	0.49	0.49
	assign (segid 3A4 and resid 363 and name CB) (segid 3A4 and resid 406 and name CA)	17.51	0.31	0.31
	assign (segid 3A4 and resid 363 and name CB) (segid 3A4 and resid 408 and name CA)	18.49	0.40	0.40
	assign (segid 3A4 and resid 363 and name CB) (segid 3A4 and resid 408 and name CB)	17.44	0.45	0.46
	assign (segid 3A4 and resid 363 and name CB) (segid 3A4 and resid 409 and name CA)	16.96	0.52	0.51
70	assign (segid 3A4 and resid 363 and name CB) (segid 3A4 and resid 409 and name CB)	15.77	0.45	0.45
	assign (segid 3A4 and resid 363 and name CB) (segid 3A4 and resid 414 and name CA)	16.81	1.21	1.20
	assign (segid 3A4 and resid 363 and name CB) (segid 3A4 and resid 415 and name CA)	16.56	1.19	1.19
	assign (segid 3A4 and resid 363 and name CB) (segid 3A4 and resid 415 and name CB)	17.24	1.31	1.31
	assign (segid 3A4 and resid 363 and name CB) (segid 3A4 and resid 425 and name CA)	15.96	2.33	2.33
75	assign (segid 3A4 and resid 363 and name CB) (segid 3A4 and resid 426 and name CA)	16.27	1.51	1.51
	assign (segid 3A4 and resid 363 and name CB) (segid 3A4 and resid 427 and name CA)	17.88	1.03	1.02
	assign (segid 3A4 and resid 363 and name CB) (segid 3A4 and resid 433 and name CA)	16.52	1.00	1.00
	assign (segid 3A4 and resid 363 and name CB) (segid 3A4 and resid 434 and name CA)	15.79	0.96	0.96
	assign (segid 3A4 and resid 363 and name CB) (segid 3A4 and resid 435 and name CA)	15.41	1.20	1.21
80	assign (segid 3A4 and resid 363 and name CB) (segid 3A4 and resid 438 and name CA)	17.20	1.07	1.07
	assign (segid 3A4 and resid 363 and name CB) (segid 3A4 and resid 364 and name C)	5.26	0.12	0.12
	assign (segid 3A4 and resid 363 and name CG) (segid 3A4 and resid 364 and name CA)	4.80	0.08	0.09

	assign (segid 3A4 and resid 363 and name CG) (segid 3A4 and resid 364 and name CB)	6.07	0.11	0.12
	assign (segid 3A4 and resid 363 and name CG) (segid 3A4 and resid 364 and name N)	3.75	0.12	0.12
	assign (segid 3A4 and resid 363 and name CG) (segid 3A4 and resid 364 and name O)	5.99	0.16	0.16
	assign (segid 3A4 and resid 363 and name CG) (segid 3A4 and resid 365 and name C)	7.61	0.15	0.15
5	assign (segid 3A4 and resid 363 and name CG) (segid 3A4 and resid 365 and name CA)	6.22	0.18	0.18
	assign (segid 3A4 and resid 363 and name CG) (segid 3A4 and resid 365 and name CB)	6.48	0.26	0.26
	assign (segid 3A4 and resid 363 and name CG) (segid 3A4 and resid 365 and name N)	5.33	0.15	0.14
	assign (segid 3A4 and resid 363 and name N) (segid 3A4 and resid 363 and name C)	2.36	0.02	0.03
	assign (segid 3A4 and resid 363 and name N) (segid 3A4 and resid 363 and name CA)	1.46	0.02	0.01
10	assign (segid 3A4 and resid 363 and name N) (segid 3A4 and resid 363 and name CB)	2.46	0.03	0.02
	assign (segid 3A4 and resid 363 and name N) (segid 3A4 and resid 363 and name CG)	3.81	0.03	0.03
	assign (segid 3A4 and resid 363 and name N) (segid 3A4 and resid 364 and name O)	2.88	0.05	0.06
	assign (segid 3A4 and resid 363 and name N) (segid 3A4 and resid 364 and name C)	5.73	0.07	0.07
	assign (segid 3A4 and resid 363 and name N) (segid 3A4 and resid 364 and name CA)	4.54	0.06	0.07
15	assign (segid 3A4 and resid 363 and name N) (segid 3A4 and resid 364 and name CB)	4.90	0.09	0.09
	assign (segid 3A4 and resid 363 and name N) (segid 3A4 and resid 364 and name N)	3.30	0.06	0.07
	assign (segid 3A4 and resid 363 and name N) (segid 3A4 and resid 364 and name O)	6.24	0.12	0.11
	assign (segid 3A4 and resid 363 and name N) (segid 3A4 and resid 365 and name CA)	7.79	0.09	0.08
	assign (segid 3A4 and resid 363 and name N) (segid 3A4 and resid 365 and name N)	6.51	0.09	0.10
20	assign (segid 3A4 and resid 363 and name O) (segid 3A4 and resid 363 and name CB)	2.91	0.09	0.08
	assign (segid 3A4 and resid 363 and name O) (segid 3A4 and resid 363 and name CG)	3.47	0.08	0.08
	assign (segid 3A4 and resid 363 and name O) (segid 3A4 and resid 364 and name C)	4.01	0.08	0.09
	assign (segid 3A4 and resid 363 and name O) (segid 3A4 and resid 364 and name CA)	2.74	0.05	0.05
	assign (segid 3A4 and resid 363 and name O) (segid 3A4 and resid 364 and name CB)	3.51	0.12	0.13
25	assign (segid 3A4 and resid 363 and name O) (segid 3A4 and resid 364 and name N)	2.23	0.02	0.02
	assign (segid 3A4 and resid 363 and name O) (segid 3A4 and resid 364 and name O)	4.97	0.04	0.05
	assign (segid 3A4 and resid 363 and name O) (segid 3A4 and resid 365 and name C)	6.83	0.09	0.10
	assign (segid 3A4 and resid 363 and name O) (segid 3A4 and resid 365 and name CA)	5.83	0.15	0.16
	assign (segid 3A4 and resid 363 and name O) (segid 3A4 and resid 365 and name CB)	6.39	0.21	0.21
30	assign (segid 3A4 and resid 363 and name O) (segid 3A4 and resid 365 and name N)	4.43	0.15	0.16
	assign (segid 3A4 and resid 364 and name C) (segid 3A4 and resid 364 and name CB)	2.51	0.03	0.02
	assign (segid 3A4 and resid 364 and name C) (segid 3A4 and resid 364 and name O)	1.24	0.02	0.01
	assign (segid 3A4 and resid 364 and name C) (segid 3A4 and resid 365 and name C)	3.06	0.05	0.05
	assign (segid 3A4 and resid 364 and name C) (segid 3A4 and resid 365 and name CA)	2.44	0.02	0.01
35	assign (segid 3A4 and resid 364 and name C) (segid 3A4 and resid 365 and name CB)	3.70	0.05	0.04
	assign (segid 3A4 and resid 364 and name C) (segid 3A4 and resid 365 and name N)	1.33	0.01	0.01
	assign (segid 3A4 and resid 364 and name C) (segid 3A4 and resid 365 and name O)	4.12	0.06	0.06
	assign (segid 3A4 and resid 364 and name CA) (segid 3A4 and resid 364 and name C)	1.51	0.01	0.01
	assign (segid 3A4 and resid 364 and name CA) (segid 3A4 and resid 364 and name CB)	1.53	0.02	0.01
40	assign (segid 3A4 and resid 364 and name CA) (segid 3A4 and resid 364 and name O)	2.39	0.02	0.01
	assign (segid 3A4 and resid 364 and name CA) (segid 3A4 and resid 365 and name C)	4.46	0.05	0.05
	assign (segid 3A4 and resid 364 and name CA) (segid 3A4 and resid 365 and name CA)	3.81	0.03	0.03
	assign (segid 3A4 and resid 364 and name CA) (segid 3A4 and resid 365 and name CB)	4.84	0.04	0.04
45	assign (segid 3A4 and resid 364 and name CA) (segid 3A4 and resid 365 and name N)	2.44	0.04	0.03
	assign (segid 3A4 and resid 364 and name CA) (segid 3A4 and resid 365 and name O)	5.58	0.06	0.05
	assign (segid 3A4 and resid 364 and name CA) (segid 3A4 and resid 381 and name CA)	13.99	0.41	0.41
	assign (segid 3A4 and resid 364 and name CA) (segid 3A4 and resid 382 and name CA)	17.08	0.33	0.33
	assign (segid 3A4 and resid 364 and name CA) (segid 3A4 and resid 382 and name CB)	18.03	0.43	0.43
	assign (segid 3A4 and resid 364 and name CA) (segid 3A4 and resid 383 and name CA)	16.38	0.37	0.37
50	assign (segid 3A4 and resid 364 and name CA) (segid 3A4 and resid 398 and name CA)	17.97	0.53	0.54
	assign (segid 3A4 and resid 364 and name CA) (segid 3A4 and resid 398 and name CB)	17.74	0.60	0.59
	assign (segid 3A4 and resid 364 and name CA) (segid 3A4 and resid 401 and name CA)	17.24	0.48	0.49
	assign (segid 3A4 and resid 364 and name CA) (segid 3A4 and resid 402 and name CA)	16.68	0.43	0.43
	assign (segid 3A4 and resid 364 and name CA) (segid 3A4 and resid 402 and name CB)	16.91	0.38	0.38
55	assign (segid 3A4 and resid 364 and name CA) (segid 3A4 and resid 405 and name CA)	16.29	0.58	0.59
	assign (segid 3A4 and resid 364 and name CA) (segid 3A4 and resid 405 and name CB)	14.91	0.60	0.60
	assign (segid 3A4 and resid 364 and name CA) (segid 3A4 and resid 406 and name CA)	17.61	0.37	0.38
	assign (segid 3A4 and resid 364 and name CA) (segid 3A4 and resid 409 and name CA)	17.83	0.54	0.53
	assign (segid 3A4 and resid 364 and name CA) (segid 3A4 and resid 409 and name CB)	16.45	0.51	0.50
60	assign (segid 3A4 and resid 364 and name CB) (segid 3A4 and resid 365 and name C)	5.08	0.11	0.10
	assign (segid 3A4 and resid 364 and name CB) (segid 3A4 and resid 365 and name CA)	4.83	0.04	0.04
	assign (segid 3A4 and resid 364 and name CB) (segid 3A4 and resid 365 and name CB)	5.98	0.08	0.09
	assign (segid 3A4 and resid 364 and name CB) (segid 3A4 and resid 365 and name N)	3.59	0.04	0.04
	assign (segid 3A4 and resid 364 and name CB) (segid 3A4 and resid 365 and name O)	6.13	0.12	0.13
65	assign (segid 3A4 and resid 364 and name CB) (segid 3A4 and resid 381 and name CA)	14.16	0.43	0.43
	assign (segid 3A4 and resid 364 and name CB) (segid 3A4 and resid 382 and name CA)	17.39	0.35	0.34
	assign (segid 3A4 and resid 364 and name CB) (segid 3A4 and resid 382 and name CB)	18.25	0.43	0.44
	assign (segid 3A4 and resid 364 and name CB) (segid 3A4 and resid 383 and name CA)	16.99	0.37	0.37
	assign (segid 3A4 and resid 364 and name CB) (segid 3A4 and resid 401 and name CA)	18.61	0.48	0.49
70	assign (segid 3A4 and resid 364 and name CB) (segid 3A4 and resid 402 and name CA)	18.00	0.45	0.45
	assign (segid 3A4 and resid 364 and name CB) (segid 3A4 and resid 402 and name CB)	18.16	0.40	0.41
	assign (segid 3A4 and resid 364 and name CB) (segid 3A4 and resid 405 and name CA)	17.76	0.59	0.60
	assign (segid 3A4 and resid 364 and name CB) (segid 3A4 and resid 405 and name CB)	16.38	0.61	0.61
	assign (segid 3A4 and resid 364 and name CB) (segid 3A4 and resid 406 and name CA)	19.00	0.41	0.40
75	assign (segid 3A4 and resid 364 and name CB) (segid 3A4 and resid 409 and name CA)	19.23	0.53	0.54
	assign (segid 3A4 and resid 364 and name CB) (segid 3A4 and resid 409 and name CB)	17.85	0.52	0.51
	assign (segid 3A4 and resid 364 and name N) (segid 3A4 and resid 364 and name C)	2.44	0.02	0.02
	assign (segid 3A4 and resid 364 and name N) (segid 3A4 and resid 364 and name CA)	1.45	0.01	0.01
	assign (segid 3A4 and resid 364 and name N) (segid 3A4 and resid 364 and name CB)	2.41	0.03	0.03
80	assign (segid 3A4 and resid 364 and name N) (segid 3A4 and resid 364 and name O)	3.05	0.07	0.07
	assign (segid 3A4 and resid 364 and name N) (segid 3A4 and resid 365 and name C)	5.48	0.07	0.06
	assign (segid 3A4 and resid 364 and name N) (segid 3A4 and resid 365 and name CA)	4.61	0.03	0.02
	assign (segid 3A4 and resid 364 and name N) (segid 3A4 and resid 365 and name CB)	5.59	0.03	0.03

	assign	(segid 3A4 and resid 361 and name N)	(segid 3A4 and resid 365 and name N)	3.33	0.02	0.02
	assign	(segid 3A4 and resid 364 and name N)	(segid 3A4 and resid 365 and name O)	6.48	0.08	0.09
	assign	(segid 3A4 and resid 364 and name O)	(segid 3A4 and resid 364 and name CB)	2.87	0.07	0.08
	assign	(segid 3A4 and resid 364 and name O)	(segid 3A4 and resid 365 and name C)	2.96	0.07	0.08
5	assign	(segid 3A4 and resid 364 and name O)	(segid 3A4 and resid 365 and name CA)	2.75	0.03	0.03
	assign	(segid 3A4 and resid 364 and name O)	(segid 3A4 and resid 365 and name CB)	4.24	0.06	0.05
	assign	(segid 3A4 and resid 364 and name O)	(segid 3A4 and resid 365 and name N)	2.24	0.03	0.02
	assign	(segid 3A4 and resid 364 and name O)	(segid 3A4 and resid 365 and name O)	3.77	0.12	0.11
	assign	(segid 3A4 and resid 364 and name O)	(segid 3A4 and resid 365 and name CB)	2.52	0.03	0.04
	assign	(segid 3A4 and resid 365 and name C)	(segid 3A4 and resid 365 and name O)	1.24	0.02	0.02
10	assign	(segid 3A4 and resid 365 and name C)	(segid 3A4 and resid 365 and name C)	1.52	0.02	0.01
	assign	(segid 3A4 and resid 365 and name CA)	(segid 3A4 and resid 365 and name CB)	1.54	0.04	0.03
	assign	(segid 3A4 and resid 365 and name CA)	(segid 3A4 and resid 365 and name O)	2.39	0.01	0.02
	assign	(segid 3A4 and resid 365 and name CA)	(segid 3A4 and resid 381 and name CA)	13.55	0.31	0.32
15	assign	(segid 3A4 and resid 365 and name CA)	(segid 3A4 and resid 382 and name CA)	16.63	0.33	0.32
	assign	(segid 3A4 and resid 365 and name CA)	(segid 3A4 and resid 382 and name CB)	17.80	0.40	0.39
	assign	(segid 3A4 and resid 365 and name CA)	(segid 3A4 and resid 383 and name CA)	15.74	0.36	0.36
	assign	(segid 3A4 and resid 365 and name CA)	(segid 3A4 and resid 384 and name CA)	18.18	0.39	0.39
	assign	(segid 3A4 and resid 365 and name CA)	(segid 3A4 and resid 384 and name CB)	17.90	0.45	0.45
20	assign	(segid 3A4 and resid 365 and name CA)	(segid 3A4 and resid 397 and name CA)	18.12	0.60	0.60
	assign	(segid 3A4 and resid 365 and name CA)	(segid 3A4 and resid 397 and name CB)	17.93	0.62	0.62
	assign	(segid 3A4 and resid 365 and name CA)	(segid 3A4 and resid 398 and name CA)	15.19	0.59	0.59
	assign	(segid 3A4 and resid 365 and name CA)	(segid 3A4 and resid 398 and name CB)	14.89	0.64	0.64
	assign	(segid 3A4 and resid 365 and name CA)	(segid 3A4 and resid 399 and name CA)	17.29	0.52	0.51
25	assign	(segid 3A4 and resid 365 and name CA)	(segid 3A4 and resid 399 and name CB)	18.71	0.53	0.52
	assign	(segid 3A4 and resid 365 and name CA)	(segid 3A4 and resid 400 and name CA)	18.11	0.52	0.52
	assign	(segid 3A4 and resid 365 and name CA)	(segid 3A4 and resid 400 and name CB)	18.91	0.46	0.46
	assign	(segid 3A4 and resid 365 and name CA)	(segid 3A4 and resid 401 and name CA)	14.63	0.53	0.52
	assign	(segid 3A4 and resid 365 and name CA)	(segid 3A4 and resid 402 and name CA)	13.51	0.52	0.52
30	assign	(segid 3A4 and resid 365 and name CA)	(segid 3A4 and resid 402 and name CB)	13.59	0.46	0.46
	assign	(segid 3A4 and resid 365 and name CA)	(segid 3A4 and resid 403 and name CA)	16.88	0.55	0.55
	assign	(segid 3A4 and resid 365 and name CA)	(segid 3A4 and resid 403 and name CB)	18.23	0.54	0.53
	assign	(segid 3A4 and resid 365 and name CA)	(segid 3A4 and resid 404 and name CA)	16.93	0.78	0.78
	assign	(segid 3A4 and resid 365 and name CA)	(segid 3A4 and resid 404 and name CB)	16.99	0.87	0.87
35	assign	(segid 3A4 and resid 365 and name CA)	(segid 3A4 and resid 405 and name CA)	13.69	0.76	0.75
	assign	(segid 3A4 and resid 365 and name CA)	(segid 3A4 and resid 405 and name CB)	12.29	0.76	0.75
	assign	(segid 3A4 and resid 365 and name CA)	(segid 3A4 and resid 406 and name CA)	14.58	0.50	0.49
	assign	(segid 3A4 and resid 365 and name CA)	(segid 3A4 and resid 407 and name CA)	18.04	0.58	0.58
	assign	(segid 3A4 and resid 365 and name CA)	(segid 3A4 and resid 408 and name CA)	17.58	0.66	0.67
40	assign	(segid 3A4 and resid 365 and name CA)	(segid 3A4 and resid 408 and name CB)	16.95	0.74	0.75
	assign	(segid 3A4 and resid 365 and name CA)	(segid 3A4 and resid 409 and name CA)	15.64	0.68	0.68
	assign	(segid 3A4 and resid 365 and name CA)	(segid 3A4 and resid 409 and name CB)	14.21	0.68	0.68
	assign	(segid 3A4 and resid 365 and name CA)	(segid 3A4 and resid 410 and name CA)	18.01	0.61	0.62
	assign	(segid 3A4 and resid 365 and name CB)	(segid 3A4 and resid 381 and name CA)	14.62	0.31	0.32
45	assign	(segid 3A4 and resid 365 and name CB)	(segid 3A4 and resid 382 and name CA)	17.56	0.33	0.33
	assign	(segid 3A4 and resid 365 and name CB)	(segid 3A4 and resid 382 and name CB)	18.79	0.38	0.37
	assign	(segid 3A4 and resid 365 and name CB)	(segid 3A4 and resid 383 and name CA)	16.44	0.37	0.37
	assign	(segid 3A4 and resid 365 and name CB)				

	assign (segid 3A4 and resid 36 and name C) (segid 3A4 and resid 350 and name CA)	5.93	0.65	0.65
	assign (segid 3A4 and resid 36 and name C) (segid 3A4 and resid 350 and name CB)	5.45	0.74	0.75
	assign (segid 3A4 and resid 36 and name C) (segid 3A4 and resid 350 and name O)	6.44	0.75	0.75
	assign (segid 3A4 and resid 36 and name C) (segid 3A4 and resid 353 and name CB)	6.49	0.60	0.59
	assign (segid 3A4 and resid 36 and name C) (segid 3A4 and resid 353 and name CG)	6.20	0.57	0.56
5	assign (segid 3A4 and resid 36 and name C) (segid 3A4 and resid 36 and name O)	1.23	0.00	0.01
	assign (segid 3A4 and resid 36 and name C) (segid 3A4 and resid 37 and name C)	3.03	0.03	0.03
	assign (segid 3A4 and resid 36 and name C) (segid 3A4 and resid 37 and name CA)	2.44	0.03	0.04
	assign (segid 3A4 and resid 36 and name C) (segid 3A4 and resid 37 and name CB)	3.68	0.04	0.04
10	assign (segid 3A4 and resid 36 and name C) (segid 3A4 and resid 37 and name N)	1.32	0.00	0.01
	assign (segid 3A4 and resid 36 and name C) (segid 3A4 and resid 37 and name O)	3.85	0.06	0.06
	assign (segid 3A4 and resid 36 and name C) (segid 3A4 and resid 38 and name C)	4.57	0.06	0.07
	assign (segid 3A4 and resid 36 and name C) (segid 3A4 and resid 38 and name CA)	4.47	0.03	0.03
	assign (segid 3A4 and resid 36 and name C) (segid 3A4 and resid 38 and name CB)	5.30	0.09	0.09
	assign (segid 3A4 and resid 36 and name C) (segid 3A4 and resid 38 and name N)	3.30	0.03	0.03
15	assign (segid 3A4 and resid 36 and name C) (segid 3A4 and resid 38 and name O)	5.66	0.10	0.09
	assign (segid 3A4 and resid 36 and name C) (segid 3A4 and resid 39 and name C)	4.85	0.11	0.11
	assign (segid 3A4 and resid 36 and name C) (segid 3A4 and resid 39 and name CA)	4.56	0.10	0.10
	assign (segid 3A4 and resid 36 and name C) (segid 3A4 and resid 39 and name CB)	4.39	0.11	0.11
	assign (segid 3A4 and resid 36 and name C) (segid 3A4 and resid 39 and name N)	3.82	0.07	0.07
20	assign (segid 3A4 and resid 36 and name C) (segid 3A4 and resid 39 and name O)	6.07	0.11	0.11
	assign (segid 3A4 and resid 36 and name C) (segid 3A4 and resid 40 and name C)	6.10	0.10	0.10
	assign (segid 3A4 and resid 36 and name C) (segid 3A4 and resid 40 and name CA)	5.05	0.11	0.12
	assign (segid 3A4 and resid 36 and name C) (segid 3A4 and resid 40 and name CB)	4.71	0.14	0.13
	assign (segid 3A4 and resid 36 and name C) (segid 3A4 and resid 40 and name N)	4.13	0.12	0.11
25	assign (segid 3A4 and resid 36 and name C) (segid 3A4 and resid 40 and name O)	7.27	0.10	0.10
	assign (segid 3A4 and resid 36 and name C) (segid 3A4 and resid 41 and name CA)	7.15	0.14	0.15
	assign (segid 3A4 and resid 36 and name C) (segid 3A4 and resid 41 and name CB)	7.12	0.19	0.19
	assign (segid 3A4 and resid 36 and name C) (segid 3A4 and resid 41 and name N)	5.91	0.13	0.12
30	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 310 and name CA)	17.01	0.55	0.55
	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 310 and name CB)	16.88	0.53	0.53
	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 311 and name CA)	16.52	0.57	0.57
	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 311 and name CB)	17.46	0.56	0.57
	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 312 and name CA)	17.98	0.65	0.64
35	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 313 and name CA)	15.59	0.58	0.58
	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 313 and name CB)	15.62	0.50	0.50
	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 314 and name CA)	12.57	0.62	0.62
	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 314 and name CB)	12.41	0.61	0.62
	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 315 and name CA)	14.44	0.71	0.70
40	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 315 and name CB)	15.73	0.68	0.69
	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 316 and name CA)	15.93	0.80	0.80
	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 317 and name CA)	13.79	0.76	0.75
	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 318 and name CA)	16.60	1.01	1.02
	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 318 and name CB)	17.69	0.95	0.95
45	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 319 and name CA)	15.37	0.96	0.96
	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 319 and name CB)	15.39	1.06	1.06
	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 322 and name CA)	15.32	0.89	0.88
	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 323 and name CA)	15.87	0.38	0.37
	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 323 and name CB)	14.74	0.40	0.40
50	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 324 and name CA)	18.47	0.37	0.36
	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 325 and name CA)	18.64	0.38	0.39
	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 325 and name CB)	18.46	0.31	0.31
	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 329 and name CA)	18.26	0.74	0.75
	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 329 and name CB)	17.33	0.69	0.69
55	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 330 and name CA)	16.69	1.03	1.02
	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 330 and name CB)	17.57	1.12	1.13
	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 331 and name CA)	12.96	1.01	1.01
	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 331 and name CB)	12.31	0.97	0.97
	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 332 and name CA)	12.16	1.21	1.20
60	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 333 and name CA)	15.70	1.03	1.02
	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 335 and name CA)	16.17	0.85	0.86
	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 336 and name CA)	18.47	0.69	0.68
	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 337 and name CA)	18.08	0.59	0.59
	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 337 and name CB)	16.87	0.53	0.53
65	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 342 and name CA)	18.14	0.31	0.32
	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 343 and name CA)	14.39	0.29	0.28
	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 343 and name CB)	13.63	0.40	0.40
	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 344 and name CA)	12.88	0.18	0.19
	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 344 and name CB)	13.61	0.30	0.30
70	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 345 and name CA)	9.47	0.29	0.28
	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 345 and name CB)	9.23	0.29	0.30
	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 346 and name CA)	9.07	0.55	0.55
	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 346 and name CB)	9.23	0.62	0.62
	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 347 and name CA)	8.28	0.61	0.61
75	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 347 and name CB)	9.38	0.63	0.64
	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 348 and name CA)	9.82	0.64	0.64
	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 349 and name C)	6.34	0.64	0.65
	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 349 and name CA)	7.51	0.71	0.71
	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 349 and name CB)	7.58	0.78	0.78
80	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 349 and name O)	6.26	0.61	0.60
	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 350 and name C)	5.28	0.68	0.68
	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 350 and name CA)	4.56	0.64	0.64
	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 350 and name CB)	4.32	0.67	0.67

	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 350 and name N)	5.64	0.63	0.62
	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 350 and name O)	5.04	0.74	0.73
	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 351 and name CA)	7.50	0.68	0.68
	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 351 and name N)	6.49	0.65	0.65
5	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 352 and name CA)	8.79	0.60	0.60
	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 352 and name CB)	9.72	0.58	0.58
	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 353 and name CA)	6.60	0.52	0.52
	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 353 and name CB)	5.17	0.59	0.60
	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 353 and name CG)	5.09	0.52	0.52
10	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 353 and name OD1)	6.21	0.49	0.50
	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 354 and name CA)	9.65	0.55	0.55
	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 354 and name CB)	10.69	0.51	0.51
	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 355 and name CA)	8.66	0.81	0.81
	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 355 and name CB)	8.00	0.84	0.83
15	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 355 and name CB)	7.76	0.83	0.82
	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 356 and name CA)	6.49	0.83	0.84
	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 357 and name CA)	10.34	0.81	0.81
	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 357 and name CB)	10.20	0.81	0.81
	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 358 and name CA)	13.65	0.81	0.81
20	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 358 and name CB)	14.77	0.84	0.84
	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 359 and name CA)	15.38	0.79	0.78
	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 359 and name CB)	16.71	0.73	0.73
	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 360 and name CA)	12.73	0.72	0.72
	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 360 and name CB)	11.47	0.77	0.76
25	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 361 and name CA)	15.47	0.69	0.70
	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 361 and name CB)	16.05	0.70	0.70
	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 362 and name CA)	17.91	0.70	0.70
	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 362 and name CB)	18.40	0.72	0.72
	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 36 and name C)	1.52	0.00	0.00
30	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 36 and name O)	2.40	0.02	0.01
	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 37 and name C)	4.43	0.04	0.03
	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 37 and name CA)	3.80	0.04	0.04
	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 37 and name CB)	4.79	0.06	0.06
	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 37 and name N)	2.42	0.03	0.02
35	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 37 and name O)	5.33	0.06	0.05
	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 381 and name CA)	8.87	0.63	0.63
	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 382 and name CA)	8.68	0.72	0.72
	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 382 and name CB)	7.53	0.75	0.75
	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 383 and name CA)	11.77	0.69	0.69
40	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 384 and name CA)	13.82	0.67	0.68
	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 384 and name CB)	14.70	0.65	0.64
	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 385 and name CA)	11.68	0.79	0.80
	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 386 and name CA)	11.23	0.77	0.76
	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 387 and name CA)	13.65	0.79	0.79
45	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 388 and name CA)	17.24	0.78	0.79
	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 389 and name CA)	17.06	0.66	0.67
	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 389 and name CB)	16.79	0.62	0.62
	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 38 and name C)	5.54	0.07	0.06
	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 38 and name CA)	5.50	0.04	0.04
50	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 38 and name CB)	6.04	0.13	0.13
	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 38 and name N)	4.42	0.04	0.05
	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 38 and name O)	6.66	0.10	0.10
	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 390 and name CA)	15.61	0.68	0.68
	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 390 and name CB)	15.38	0.69	0.70
55	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 391 and name CA)	17.83	0.71	0.72
	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 391 and name CB)	17.53	0.74	0.74
	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 394 and name CB)	18.73	0.81	0.82
	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 39 and name C)	5.64	0.20	0.19
	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 39 and name CA)	5.12	0.14	0.14
60	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 39 and name CB)	4.50	0.17	0.17
	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 39 and name N)	4.57	0.08	0.08
	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 39 and name O)	6.84	0.21	0.20
	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 40 and name C)	7.29	0.15	0.16
	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 40 and name CA)	6.11	0.20	0.20
65	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 40 and name CB)	5.84	0.20	0.21
	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 40 and name N)	5.10	0.19	0.19
	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 41 and name CA)	8.49	0.13	0.14
	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 41 and name CB)	8.50	0.14	0.15
	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 41 and name N)	7.21	0.13	0.14
70	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 42 and name CA)	9.89	0.23	0.24
	assign (segid 3A4 and resid 36 and name CA) (segid 3A4 and resid 42 and name CB)	9.52	0.25	0.25
	assign (segid 3A4 and resid 36 and name N) (segid 3A4 and resid 349 and name C)	5.92	0.45	0.45
	assign (segid 3A4 and resid 36 and name N) (segid 3A4 and resid 349 and name O)	5.73	0.43	0.44
	assign (segid 3A4 and resid 36 and name N) (segid 3A4 and resid 350 and name C)	5.44	0.62	0.62
75	assign (segid 3A4 and resid 36 and name N) (segid 3A4 and resid 350 and name CA)	4.60	0.53	0.53
	assign (segid 3A4 and resid 36 and name N) (segid 3A4 and resid 350 and name CB)	4.73	0.57	0.56
	assign (segid 3A4 and resid 36 and name N) (segid 3A4 and resid 350 and name N)	5.45	0.44	0.45
	assign (segid 3A4 and resid 36 and name N) (segid 3A4 and resid 350 and name O)	5.24	0.74	0.73
	assign (segid 3A4 and resid 36 and name N) (segid 3A4 and resid 353 and name CA)	6.04	0.61	0.60
80	assign (segid 3A4 and resid 36 and name N) (segid 3A4 and resid 353 and name CB)	4.67	0.74	0.73
	assign (segid 3A4 and resid 36 and name N) (segid 3A4 and resid 353 and name CG)	4.37	0.72	0.72
	assign (segid 3A4 and resid 36 and name N) (segid 3A4 and resid 353 and name OD1)	5.47	0.72	0.71
	assign (segid 3A4 and resid 36 and name N) (segid 3A4 and resid 36 and name C)	2.44	0.03	0.04

	assign (segid 3A4 and resid 36 and name N) (segid 3A4 and resid 36 and name CA)	1.45	0.01	0.01
	assign (segid 3A4 and resid 36 and name N) (segid 3A4 and resid 36 and name O)	3.49	0.04	0.04
	assign (segid 3A4 and resid 36 and name N) (segid 3A4 and resid 37 and name C)	4.73	0.09	0.10
	assign (segid 3A4 and resid 36 and name N) (segid 3A4 and resid 37 and name CA)	4.18	0.08	0.09
5	assign (segid 3A4 and resid 36 and name N) (segid 3A4 and resid 37 and name CB)	4.85	0.15	0.14
	assign (segid 3A4 and resid 36 and name N) (segid 3A4 and resid 37 and name N)	2.78	0.08	0.08
	assign (segid 3A4 and resid 36 and name N) (segid 3A4 and resid 37 and name O)	5.81	0.10	0.10
	assign (segid 3A4 and resid 36 and name N) (segid 3A4 and resid 38 and name C)	5.69	0.07	0.08
	assign (segid 3A4 and resid 36 and name N) (segid 3A4 and resid 38 and name CA)	5.42	0.12	0.13
	assign (segid 3A4 and resid 36 and name N) (segid 3A4 and resid 38 and name CB)	5.61	0.23	0.23
10	assign (segid 3A4 and resid 36 and name N) (segid 3A4 and resid 38 and name N)	4.39	0.12	0.12
	assign (segid 3A4 and resid 36 and name N) (segid 3A4 and resid 38 and name O)	6.89	0.06	0.06
	assign (segid 3A4 and resid 36 and name N) (segid 3A4 and resid 39 and name C)	6.39	0.14	0.14
	assign (segid 3A4 and resid 36 and name N) (segid 3A4 and resid 39 and name CA)	5.58	0.10	0.11
	assign (segid 3A4 and resid 36 and name N) (segid 3A4 and resid 39 and name CB)	5.00	0.18	0.17
15	assign (segid 3A4 and resid 36 and name N) (segid 3A4 and resid 39 and name N)	4.83	0.06	0.07
	assign (segid 3A4 and resid 36 and name N) (segid 3A4 and resid 39 and name O)	7.59	0.14	0.14
	assign (segid 3A4 and resid 36 and name N) (segid 3A4 and resid 40 and name CA)	7.19	0.14	0.14
	assign (segid 3A4 and resid 36 and name N) (segid 3A4 and resid 40 and name CB)	7.04	0.15	0.15
	assign (segid 3A4 and resid 36 and name N) (segid 3A4 and resid 40 and name N)	6.05	0.14	0.14
20	assign (segid 3A4 and resid 36 and name N) (segid 3A4 and resid 350 and name CB)	5.57	0.86	0.85
	assign (segid 3A4 and resid 36 and name O) (segid 3A4 and resid 37 and name C)	2.98	0.04	0.04
	assign (segid 3A4 and resid 36 and name O) (segid 3A4 and resid 37 and name CA)	2.79	0.03	0.04
	assign (segid 3A4 and resid 36 and name O) (segid 3A4 and resid 37 and name CB)	4.25	0.04	0.05
	assign (segid 3A4 and resid 36 and name O) (segid 3A4 and resid 37 and name N)	2.25	0.01	0.01
25	assign (segid 3A4 and resid 36 and name O) (segid 3A4 and resid 37 and name O)	3.44	0.08	0.08
	assign (segid 3A4 and resid 36 and name O) (segid 3A4 and resid 38 and name C)	4.13	0.11	0.11
	assign (segid 3A4 and resid 36 and name O) (segid 3A4 and resid 38 and name CA)	4.37	0.07	0.07
	assign (segid 3A4 and resid 36 and name O) (segid 3A4 and resid 38 and name CB)	5.43	0.12	0.11
	assign (segid 3A4 and resid 36 and name O) (segid 3A4 and resid 38 and name N)	3.43	0.05	0.05
30	assign (segid 3A4 and resid 36 and name O) (segid 3A4 and resid 38 and name O)	5.06	0.13	0.14
	assign (segid 3A4 and resid 36 and name O) (segid 3A4 and resid 39 and name C)	3.84	0.12	0.11
	assign (segid 3A4 and resid 36 and name O) (segid 3A4 and resid 39 and name CA)	3.83	0.15	0.15
	assign (segid 3A4 and resid 36 and name O) (segid 3A4 and resid 39 and name CB)	3.80	0.18	0.18
	assign (segid 3A4 and resid 36 and name O) (segid 3A4 and resid 39 and name N)	3.34	0.13	0.13
35	assign (segid 3A4 and resid 36 and name O) (segid 3A4 and resid 39 and name O)	5.02	0.12	0.12
	assign (segid 3A4 and resid 36 and name O) (segid 3A4 and resid 40 and name C)	4.97	0.11	0.12
	assign (segid 3A4 and resid 36 and name O) (segid 3A4 and resid 40 and name CA)	3.85	0.11	0.12
	assign (segid 3A4 and resid 36 and name O) (segid 3A4 and resid 40 and name CB)	3.59	0.15	0.15
	assign (segid 3A4 and resid 36 and name O) (segid 3A4 and resid 40 and name N)	2.98	0.12	0.13
40	assign (segid 3A4 and resid 36 and name O) (segid 3A4 and resid 40 and name O)	6.12	0.12	0.11
	assign (segid 3A4 and resid 36 and name O) (segid 3A4 and resid 41 and name C)	7.17	0.17	0.16
	assign (segid 3A4 and resid 36 and name O) (segid 3A4 and resid 41 and name CA)	6.26	0.15	0.15
	assign (segid 3A4 and resid 36 and name O) (segid 3A4 and resid 41 and name CB)	6.43	0.18	0.17
	assign (segid 3A4 and resid 36 and name O) (segid 3A4 and resid 41 and name N)	4.92	0.14	0.14
45	assign (segid 3A4 and resid 36 and name O) (segid 3A4 and resid 42 and name N)	6.90	0.20	0.20
	assign (segid 3A4 and resid 37 and name C) (segid 3A4 and resid 37 and name CB)	2.51	0.02	0.02
	assign (segid 3A4 and resid 37 and name C) (segid 3A4 and resid 37 and name O)	1.23	0.01	0.01
	assign (segid 3A4 and resid 37 and name C) (segid 3A4 and resid 38 and name C)	3.12	0.09	0.08
50	assign (segid 3A4 and resid 37 and name C) (segid 3A4 and resid 38 and name CA)	2.43	0.01	0.01
	assign (segid 3A4 and resid 37 and name C) (segid 3A4 and resid 38 and name CB)	3.67	0.03	0.03
	assign (segid 3A4 and resid 37 and name C) (segid 3A4 and resid 38 and name N)	1.32	0.01	0.01
	assign (segid 3A4 and resid 37 and name C) (segid 3A4 and resid 38 and name O)	4.00	0.11	0.11
	assign (segid 3A4 and resid 37 and name C) (segid 3A4 and resid 39 and name C)	4.68	0.11	0.12
55	assign (segid 3A4 and resid 37 and name C) (segid 3A4 and resid 39 and name CA)	4.59	0.12	0.13
	assign (segid 3A4 and resid 37 and name C) (segid 3A4 and resid 39 and name CB)	5.36	0.12	0.11
	assign (segid 3A4 and resid 37 and name C) (segid 3A4 and resid 39 and name N)	3.38	0.11	0.10
	assign (segid 3A4 and resid 37 and name C) (segid 3A4 and resid 39 and name O)	5.72	0.12	0.13
	assign (segid 3A4 and resid 37 and name C) (segid 3A4 and resid 40 and name C)	5.08	0.20	0.21
	assign (segid 3A4 and resid 37 and name C) (segid 3A4 and resid 40 and name CA)	4.80	0.16	0.16
60	assign (segid 3A4 and resid 37 and name C) (segid 3A4 and resid 40 and name CB)	4.63	0.18	0.17
	assign (segid 3A4 and resid 37 and name C) (segid 3A4 and resid 40 and name N)	4.05	0.12	0.12
	assign (segid 3A4 and resid 37 and name C) (segid 3A4 and resid 40 and name O)	6.28	0.20	0.20
	assign (segid 3A4 and resid 37 and name C) (segid 3A4 and resid 41 and name C)	6.21	0.27	0.26
	assign (segid 3A4 and resid 37 and name C) (segid 3A4 and resid 41 and name CA)	5.11	0.28	0.29
65	assign (segid 3A4 and resid 37 and name C) (segid 3A4 and resid 41 and name CB)	4.61	0.32	0.31
	assign (segid 3A4 and resid 37 and name C) (segid 3A4 and resid 41 and name N)	4.30	0.26	0.25
	assign (segid 3A4 and resid 37 and name C) (segid 3A4 and resid 41 and name O)	7.36	0.27	0.27
	assign (segid 3A4 and resid 37 and name C) (segid 3A4 and resid 42 and name CA)	7.38	0.25	0.24
	assign (segid 3A4 and resid 37 and name C) (segid 3A4 and resid 42 and name CB)	7.39	0.23	0.23
70	assign (segid 3A4 and resid 37 and name C) (segid 3A4 and resid 42 and name N)	6.10	0.25	0.25
	assign (segid 3A4 and resid 37 and name C) (segid 3A4 and resid 313 and name CB)	18.80	0.68	0.69
	assign (segid 3A4 and resid 37 and name CA) (segid 3A4 and resid 314 and name CA)	16.01	0.74	0.73
	assign (segid 3A4 and resid 37 and name CA) (segid 3A4 and resid 314 and name CB)	15.75	0.76	0.76
	assign (segid 3A4 and resid 37 and name CA) (segid 3A4 and resid 315 and name CA)	18.07	0.74	0.74
75	assign (segid 3A4 and resid 37 and name CA) (segid 3A4 and resid 317 and name CA)	17.34	0.82	0.83
	assign (segid 3A4 and resid 37 and name CA) (segid 3A4 and resid 322 and name CA)	16.48	0.94	0.94
	assign (segid 3A4 and resid 37 and name CA) (segid 3A4 and resid 323 and name CA)	16.21	0.37	0.36
	assign (segid 3A4 and resid 37 and name CA) (segid 3A4 and resid 323 and name CB)	14.90	0.33	0.33
	assign (segid 3A4 and resid 37 and name CA) (segid 3A4 and resid 324 and name CA)	18.25	0.25	0.26
80	assign (segid 3A4 and resid 37 and name CA) (segid 3A4 and resid 325 and name CA)	17.69	0.34	0.33
	assign (segid 3A4 and resid 37 and name CA) (segid 3A4 and resid 325 and name CB)	17.36	0.31	0.31
	assign (segid 3A4 and resid 37 and name CA) (segid 3A4 and resid 329 and name CA)	16.01	0.78	0.78

	assign (segid 3A4 and resid 37 and name CA) (segid 3A4 and resid 329 and name CB)	15.20	0.71	0.71
	assign (segid 3A4 and resid 37 and name CA) (segid 3A4 and resid 330 and name CA)	14.13	1.05	1.05
	assign (segid 3A4 and resid 37 and name CA) (segid 3A4 and resid 330 and name CB)	14.83	1.18	1.17
	assign (segid 3A4 and resid 37 and name CA) (segid 3A4 and resid 331 and name CA)	10.52	0.97	0.98
5	assign (segid 3A4 and resid 37 and name CA) (segid 3A4 and resid 331 and name CB)	10.21	0.91	0.90
	assign (segid 3A4 and resid 37 and name CA) (segid 3A4 and resid 332 and name CA)	9.47	1.19	1.20
	assign (segid 3A4 and resid 37 and name CA) (segid 3A4 and resid 333 and name CA)	13.09	1.13	1.13
	assign (segid 3A4 and resid 37 and name CA) (segid 3A4 and resid 335 and name CA)	14.20	0.88	0.87
	assign (segid 3A4 and resid 37 and name CA) (segid 3A4 and resid 336 and name CA)	16.45	0.76	0.76
10	assign (segid 3A4 and resid 37 and name CA) (segid 3A4 and resid 336 and name CB)	17.79	0.80	0.80
	assign (segid 3A4 and resid 37 and name CA) (segid 3A4 and resid 337 and name CA)	16.57	0.58	0.59
	assign (segid 3A4 and resid 37 and name CA) (segid 3A4 and resid 337 and name CB)	15.44	0.53	0.53
	assign (segid 3A4 and resid 37 and name CA) (segid 3A4 and resid 341 and name CB)	18.75	0.44	0.44
	assign (segid 3A4 and resid 37 and name CA) (segid 3A4 and resid 342 and name CA)	18.31	0.34	0.34
15	assign (segid 3A4 and resid 37 and name CA) (segid 3A4 and resid 343 and name CA)	14.72	0.27	0.28
	assign (segid 3A4 and resid 37 and name CA) (segid 3A4 and resid 343 and name CB)	13.69	0.36	0.36
	assign (segid 3A4 and resid 37 and name CA) (segid 3A4 and resid 344 and name CA)	14.17	0.18	0.18
	assign (segid 3A4 and resid 37 and name CA) (segid 3A4 and resid 344 and name CB)	15.11	0.25	0.24
	assign (segid 3A4 and resid 37 and name CA) (segid 3A4 and resid 345 and name CA)	11.09	0.41	0.42
20	assign (segid 3A4 and resid 37 and name CA) (segid 3A4 and resid 345 and name CB)	10.67	0.51	0.50
	assign (segid 3A4 and resid 37 and name CA) (segid 3A4 and resid 346 and name CA)	11.72	0.53	0.54
	assign (segid 3A4 and resid 37 and name CA) (segid 3A4 and resid 346 and name CB)	11.92	0.52	0.52
	assign (segid 3A4 and resid 37 and name CA) (segid 3A4 and resid 347 and name CA)	11.38	0.70	0.70
	assign (segid 3A4 and resid 37 and name CA) (segid 3A4 and resid 347 and name CB)	12.38	0.78	0.77
25	assign (segid 3A4 and resid 37 and name CA) (segid 3A4 and resid 348 and name CA)	13.38	0.60	0.60
	assign (segid 3A4 and resid 37 and name CA) (segid 3A4 and resid 349 and name CA)	11.08	0.52	0.52
	assign (segid 3A4 and resid 37 and name CA) (segid 3A4 and resid 349 and name CB)	10.78	0.59	0.58
	assign (segid 3A4 and resid 37 and name CA) (segid 3A4 and resid 350 and name CA)	8.24	0.57	0.58
	assign (segid 3A4 and resid 37 and name CA) (segid 3A4 and resid 350 and name CB)	7.82	0.70	0.69
30	assign (segid 3A4 and resid 37 and name CA) (segid 3A4 and resid 351 and name CA)	11.12	0.72	0.71
	assign (segid 3A4 and resid 37 and name CA) (segid 3A4 and resid 352 and name CA)	12.29	0.55	0.55
	assign (segid 3A4 and resid 37 and name CA) (segid 3A4 and resid 352 and name CB)	13.25	0.50	0.51
	assign (segid 3A4 and resid 37 and name CA) (segid 3A4 and resid 353 and name CA)	9.53	0.57	0.57
	assign (segid 3A4 and resid 37 and name CA) (segid 3A4 and resid 353 and name CB)	8.06	0.64	0.65
35	assign (segid 3A4 and resid 37 and name CA) (segid 3A4 and resid 354 and name CA)	11.84	0.71	0.71
	assign (segid 3A4 and resid 37 and name CA) (segid 3A4 and resid 354 and name CB)	12.74	0.67	0.67
	assign (segid 3A4 and resid 37 and name CA) (segid 3A4 and resid 355 and name CA)	9.77	1.12	1.12
	assign (segid 3A4 and resid 37 and name CA) (segid 3A4 and resid 355 and name CB)	8.68	1.17	1.17
	assign (segid 3A4 and resid 37 and name CA) (segid 3A4 and resid 356 and name CA)	9.44	1.06	1.06
40	assign (segid 3A4 and resid 37 and name CA) (segid 3A4 and resid 356 and name CB)	8.47	1.03	1.04
	assign (segid 3A4 and resid 37 and name CA) (segid 3A4 and resid 357 and name CA)	12.77	0.97	0.96
	assign (segid 3A4 and resid 37 and name CA) (segid 3A4 and resid 357 and name CB)	12.96	0.92	0.92
	assign (segid 3A4 and resid 37 and name CA) (segid 3A4 and resid 358 and name CA)	15.79	0.86	0.87
	assign (segid 3A4 and resid 37 and name CA) (segid 3A4 and resid 358 and name CB)	16.71	0.95	0.94
45	assign (segid 3A4 and resid 37 and name CA) (segid 3A4 and resid 359 and name CA)	18.07	0.82	0.82
	assign (segid 3A4 and resid 37 and name CA) (segid 3A4 and resid 360 and name CA)	15.86	0.72	0.72
	assign (segid 3A4 and resid 37 and name CA) (segid 3A4 and resid 360 and name CB)	14.59	0.72	0.72
	assign (segid 3A4 and resid 37 and name CA) (segid 3A4 and resid 37 and name C)	1.52	0.00	0.01
	assign (segid 3A4 and resid 37 and name CA) (segid 3A4 and resid 37 and name CB)	1.52	0.01	0.02
50	assign (segid 3A4 and resid 37 and name CA) (segid 3A4 and resid 37 and name O)	2.39	0.02	0.01
	assign (segid 3A4 and resid 37 and name CA) (segid 3A4 and resid 381 and name CA)	11.60	0.71	0.72
	assign (segid 3A4 and resid 37 and name CA) (segid 3A4 and resid 382 and name CA)	11.29	0.95	0.96
	assign (segid 3A4 and resid 37 and name CA) (segid 3A4 and resid 382 and name CB)	10.07	0.97	0.97
	assign (segid 3A4 and resid 37 and name CA) (segid 3A4 and resid 383 and name CA)	14.73	0.88	0.88
55	assign (segid 3A4 and resid 37 and name CA) (segid 3A4 and resid 384 and name CA)	16.16	0.97	0.97
	assign (segid 3A4 and resid 37 and name CA) (segid 3A4 and resid 384 and name CB)	16.91	0.98	0.98
	assign (segid 3A4 and resid 37 and name CA) (segid 3A4 and resid 385 and name CA)	13.53	1.09	1.10
	assign (segid 3A4 and resid 37 and name CA) (segid 3A4 and resid 386 and name CA)	12.07	1.24	1.24
	assign (segid 3A4 and resid 37 and name CA) (segid 3A4 and resid 387 and name CA)	13.63	1.35	1.36
60	assign (segid 3A4 and resid 37 and name CA) (segid 3A4 and resid 38 and name C)	4.49	0.07	0.07
	assign (segid 3A4 and resid 37 and name CA) (segid 3A4 and resid 38 and name CA)	3.80	0.01	0.02
	assign (segid 3A4 and resid 37 and name CA) (segid 3A4 and resid 38 and name CB)	4.83	0.03	0.03
	assign (segid 3A4 and resid 37 and name CA) (segid 3A4 and resid 38 and name N)	2.43	0.02	0.02
	assign (segid 3A4 and resid 37 and name CA) (segid 3A4 and resid 38 and name O)	5.46	0.10	0.09
65	assign (segid 3A4 and resid 37 and name CA) (segid 3A4 and resid 390 and name CA)	16.74	1.11	1.11
	assign (segid 3A4 and resid 37 and name CA) (segid 3A4 and resid 390 and name CB)	16.38	1.12	1.12
	assign (segid 3A4 and resid 37 and name CA) (segid 3A4 and resid 39 and name C)	5.63	0.11	0.11
	assign (segid 3A4 and resid 37 and name CA) (segid 3A4 and resid 39 and name CA)	5.56	0.10	0.10
	assign (segid 3A4 and resid 37 and name CA) (segid 3A4 and resid 39 and name CB)	6.00	0.09	0.09
70	assign (segid 3A4 and resid 37 and name CA) (segid 3A4 and resid 39 and name N)	4.44	0.07	0.08
	assign (segid 3A4 and resid 37 and name CA) (segid 3A4 and resid 39 and name O)	6.74	0.13	0.13
	assign (segid 3A4 and resid 37 and name CA) (segid 3A4 and resid 40 and name C)	5.96	0.23	0.23
	assign (segid 3A4 and resid 37 and name CA) (segid 3A4 and resid 40 and name CA)	5.42	0.18	0.18
	assign (segid 3A4 and resid 37 and name CA) (segid 3A4 and resid 40 and name CB)	4.87	0.20	0.19
	assign (segid 3A4 and resid 37 and name CA) (segid 3A4 and resid 40 and name N)	4.79	0.13	0.13
75	assign (segid 3A4 and resid 37 and name CA) (segid 3A4 and resid 40 and name O)	7.15	0.22	0.22
	assign (segid 3A4 and resid 37 and name CA) (segid 3A4 and resid 41 and name CA)	6.30	0.34	0.34
	assign (segid 3A4 and resid 37 and name CA) (segid 3A4 and resid 41 and name CB)	5.88	0.39	0.39
	assign (segid 3A4 and resid 37 and name CA) (segid 3A4 and resid 41 and name N)	5.36	0.30	0.31
80	assign (segid 3A4 and resid 37 and name CA) (segid 3A4 and resid 42 and name CA)	8.77	0.25	0.24
	assign (segid 3A4 and resid 37 and name CA) (segid 3A4 and resid 42 and name CB)	8.80	0.21	0.20
	assign (segid 3A4 and resid 37 and name CA) (segid 3A4 and resid 42 and name N)	7.46	0.26	0.27
	assign (segid 3A4 and resid 37 and name CB) (segid 3A4 and resid 314 and name CA)	16.98	0.69	0.70

	assign (segid 3A4 and resid 37 and name CB) (segid 3A4 and resid 314 and name CB)	16.65	0.72	0.72
	assign (segid 3A4 and resid 37 and name CB) (segid 3A4 and resid 317 and name CA)	18.47	0.72	0.73
	assign (segid 3A4 and resid 37 and name CB) (segid 3A4 and resid 322 and name CA)	17.67	0.95	0.96
	assign (segid 3A4 and resid 37 and name CB) (segid 3A4 and resid 323 and name CA)	17.32	0.41	0.41
5	assign (segid 3A4 and resid 37 and name CB) (segid 3A4 and resid 323 and name CB)	16.02	0.37	0.37
	assign (segid 3A4 and resid 37 and name CB) (segid 3A4 and resid 324 and name CA)	19.20	0.29	0.28
	assign (segid 3A4 and resid 37 and name CB) (segid 3A4 and resid 325 and name CA)	18.44	0.33	0.33
	assign (segid 3A4 and resid 37 and name CB) (segid 3A4 and resid 325 and name CB)	18.01	0.30	0.31
	assign (segid 3A4 and resid 37 and name CB) (segid 3A4 and resid 329 and name CA)	16.22	0.79	0.79
	assign (segid 3A4 and resid 37 and name CB) (segid 3A4 and resid 329 and name CB)	15.54	0.72	0.72
10	assign (segid 3A4 and resid 37 and name CB) (segid 3A4 and resid 330 and name CA)	14.04	1.05	1.06
	assign (segid 3A4 and resid 37 and name CB) (segid 3A4 and resid 330 and name CB)	14.61	1.19	1.19
	assign (segid 3A4 and resid 37 and name CB) (segid 3A4 and resid 331 and name CA)	10.47	0.97	0.96
	assign (segid 3A4 and resid 37 and name CB) (segid 3A4 and resid 331 and name CB)	10.32	0.90	0.90
	assign (segid 3A4 and resid 37 and name CB) (segid 3A4 and resid 332 and name CA)	8.96	1.13	1.13
15	assign (segid 3A4 and resid 37 and name CB) (segid 3A4 and resid 333 and name CA)	12.47	1.07	1.07
	assign (segid 3A4 and resid 37 and name CB) (segid 3A4 and resid 335 and name CA)	13.86	0.87	0.87
	assign (segid 3A4 and resid 37 and name CB) (segid 3A4 and resid 336 and name CA)	16.32	0.78	0.78
	assign (segid 3A4 and resid 37 and name CB) (segid 3A4 and resid 336 and name CB)	17.60	0.82	0.83
	assign (segid 3A4 and resid 37 and name CB) (segid 3A4 and resid 337 and name CA)	16.78	0.61	0.61
20	assign (segid 3A4 and resid 37 and name CB) (segid 3A4 and resid 337 and name CB)	15.74	0.55	0.55
	assign (segid 3A4 and resid 37 and name CB) (segid 3A4 and resid 341 and name CB)	19.28	0.45	0.44
	assign (segid 3A4 and resid 37 and name CB) (segid 3A4 and resid 342 and name CA)	19.11	0.43	0.42
	assign (segid 3A4 and resid 37 and name CB) (segid 3A4 and resid 343 and name CA)	15.56	0.37	0.38
	assign (segid 3A4 and resid 37 and name CB) (segid 3A4 and resid 343 and name CB)	14.53	0.44	0.43
25	assign (segid 3A4 and resid 37 and name CB) (segid 3A4 and resid 344 and name CA)	15.15	0.23	0.22
	assign (segid 3A4 and resid 37 and name CB) (segid 3A4 and resid 344 and name CB)	16.03	0.26	0.27
	assign (segid 3A4 and resid 37 and name CB) (segid 3A4 and resid 345 and name CA)	12.21	0.36	0.37
	assign (segid 3A4 and resid 37 and name CB) (segid 3A4 and resid 345 and name CB)	11.88	0.48	0.48
	assign (segid 3A4 and resid 37 and name CB) (segid 3A4 and resid 346 and name CA)	12.77	0.39	0.40
30	assign (segid 3A4 and resid 37 and name CB) (segid 3A4 and resid 346 and name CB)	12.84	0.39	0.38
	assign (segid 3A4 and resid 37 and name CB) (segid 3A4 and resid 347 and name CA)	12.60	0.55	0.55
	assign (segid 3A4 and resid 37 and name CB) (segid 3A4 and resid 347 and name CB)	13.67	0.64	0.64
	assign (segid 3A4 and resid 37 and name CB) (segid 3A4 and resid 348 and name CA)	14.37	0.40	0.40
	assign (segid 3A4 and resid 37 and name CB) (segid 3A4 and resid 349 and name CA)	11.81	0.36	0.36
35	assign (segid 3A4 and resid 37 and name CB) (segid 3A4 and resid 349 and name CB)	11.46	0.47	0.46
	assign (segid 3A4 and resid 37 and name CB) (segid 3A4 and resid 350 and name CA)	9.15	0.47	0.47
	assign (segid 3A4 and resid 37 and name CB) (segid 3A4 and resid 350 and name CB)	8.90	0.58	0.59
	assign (segid 3A4 and resid 37 and name CB) (segid 3A4 and resid 351 and name CA)	11.97	0.70	0.69
	assign (segid 3A4 and resid 37 and name CB) (segid 3A4 and resid 352 and name CA)	12.78	0.58	0.58
40	assign (segid 3A4 and resid 37 and name CB) (segid 3A4 and resid 352 and name CB)	13.74	0.53	0.54
	assign (segid 3A4 and resid 37 and name CB) (segid 3A4 and resid 353 and name CA)	9.71	0.65	0.66
	assign (segid 3A4 and resid 37 and name CB) (segid 3A4 and resid 353 and name CB)	8.30	0.72	0.72
	assign (segid 3A4 and resid 37 and name CB) (segid 3A4 and resid 354 and name CA)	11.63	0.82	0.83
	assign (segid 3A4 and resid 37 and name CB) (segid 3A4 and resid 354 and name CB)	12.42	0.79	0.79
45	assign (segid 3A4 and resid 37 and name CB) (segid 3A4 and resid 355 and name CA)	9.29	1.25	1.26
	assign (segid 3A4 and resid 37 and name CB) (segid 3A4 and resid 355 and name CB)	8.07	1.31	1.30
	assign (segid 3A4 and resid 37 and name CB) (segid 3A4 and resid 356 and name CA)	9.47	1.15	1.15
	assign (segid 3A4 and resid 37 and name CB) (segid 3A4 and resid 356 and name CB)	8.72	1.10	1.09
50	assign (segid 3A4 and resid 37 and name CB) (segid 3A4 and resid 357 and name CA)	12.94	1.04	1.03
	assign (segid 3A4 and resid 37 and name CB) (segid 3A4 and resid 357 and name CB)	13.27	0.98	0.97
	assign (segid 3A4 and resid 37 and name CB) (segid 3A4 and resid 358 and name CA)	15.65	0.87	0.88
	assign (segid 3A4 and resid 37 and name CB) (segid 3A4 and resid 358 and name CB)	16.50	0.98	0.98
	assign (segid 3A4 and resid 37 and name CB) (segid 3A4 and resid 359 and name CA)	18.07	0.83	0.82
	assign (segid 3A4 and resid 37 and name CB) (segid 3A4 and resid 360 and name CA)	16.11	0.71	0.72
55	assign (segid 3A4 and resid 37 and name CB) (segid 3A4 and resid 360 and name CB)	14.82	0.71	0.70
	assign (segid 3A4 and resid 37 and name CB) (segid 3A4 and resid 381 and name CA)	12.71	0.73	0.74
	assign (segid 3A4 and resid 37 and name CB) (segid 3A4 and resid 382 and name CA)	12.64	0.93	0.93
	assign (segid 3A4 and resid 37 and name CB) (segid 3A4 and resid 382 and name CB)	11.46	0.94	0.93
	assign (segid 3A4 and resid 37 and name CB) (segid 3A4 and resid 383 and name CA)	16.06	0.82	0.82
60	assign (segid 3A4 and resid 37 and name CB) (segid 3A4 and resid 384 and name CA)	17.58	0.92	0.93
	assign (segid 3A4 and resid 37 and name CB) (segid 3A4 and resid 385 and name CA)	15.00	1.05	1.05
	assign (segid 3A4 and resid 37 and name CB) (segid 3A4 and resid 386 and name CA)	13.50	1.25	1.25
	assign (segid 3A4 and resid 37 and name CB) (segid 3A4 and resid 387 and name CA)	14.97	1.42	1.42
65	assign (segid 3A4 and resid 37 and name CB) (segid 3A4 and resid 38 and name C)	5.49	0.06	0.06
	assign (segid 3A4 and resid 37 and name CB) (segid 3A4 and resid 38 and name CB)	4.46	0.04	0.03
	assign (segid 3A4 and resid 37 and name CB) (segid 3A4 and resid 38 and name N)	3.13	0.04	0.05
	assign (segid 3A4 and resid 37 and name CB) (segid 3A4 and resid 38 and name O)	6.43	0.11	0.10
	assign (segid 3A4 and resid 37 and name CB) (segid 3A4 and resid 39 and name C)	7.03	0.10	0.09
70	assign (segid 3A4 and resid 37 and name CB) (segid 3A4 and resid 39 and name CA)	6.88	0.07	0.06
	assign (segid 3A4 and resid 37 and name CB) (segid 3A4 and resid 39 and name CB)	7.34	0.05	0.06
	assign (segid 3A4 and resid 37 and name CB) (segid 3A4 and resid 39 and name N)	5.64	0.06	0.05
	assign (segid 3A4 and resid 37 and name CB) (segid 3A4 and resid 40 and name C)	7.21	0.30	0.30
	assign (segid 3A4 and resid 37 and name CB) (segid 3A4 and resid 40 and name CA)	6.82	0.22	0.22
75	assign (segid 3A4 and resid 37 and name CB) (segid 3A4 and resid 40 and name CB)	6.20	0.26	0.27
	assign (segid 3A4 and resid 37 and name CB) (segid 3A4 and resid 40 and name N)	6.24	0.14	0.13
	assign (segid 3A4 and resid 37 and name CB) (segid 3A4 and resid 41 and name CA)	7.19	0.45	0.46
	assign (segid 3A4 and resid 37 and name CB) (segid 3A4 and resid 41 and name CB)	6.52	0.52	0.52
	assign (segid 3A4 and resid 37 and name CB) (segid 3A4 and resid 41 and name N)	6.47	0.38	0.39
80	assign (segid 3A4 and resid 37 and name CB) (segid 3A4 and resid 42 and name CA)	9.79	0.29	0.29
	assign (segid 3A4 and resid 37 and name CB) (segid 3A4 and resid 42 and name CB)	9.83	0.22	0.21
	assign (segid 3A4 and resid 37 and name N) (segid 3A4 and resid 353 and name CG)	6.11	0.66	0.67

	assign (segid 3A4 and resid 37 and name N) (segid 3A4 and resid 37 and name C)	2.46	0.01	0.01
	assign (segid 3A4 and resid 37 and name N) (segid 3A4 and resid 37 and name CA)	1.46	0.02	0.01
	assign (segid 3A4 and resid 37 and name N) (segid 3A4 and resid 37 and name CB)	2.42	0.04	0.04
	assign (segid 3A4 and resid 37 and name N) (segid 3A4 and resid 37 and name O)	3.49	0.02	0.02
	assign (segid 3A4 and resid 37 and name N) (segid 3A4 and resid 38 and name C)	4.74	0.04	0.05
5	assign (segid 3A4 and resid 37 and name N) (segid 3A4 and resid 38 and name CA)	4.22	0.02	0.03
	assign (segid 3A4 and resid 37 and name N) (segid 3A4 and resid 38 and name CB)	5.00	0.05	0.06
	assign (segid 3A4 and resid 37 and name N) (segid 3A4 and resid 38 and name N)	2.83	0.03	0.03
	assign (segid 3A4 and resid 37 and name N) (segid 3A4 and resid 38 and name O)	5.86	0.08	0.07
	assign (segid 3A4 and resid 37 and name N) (segid 3A4 and resid 39 and name C)	5.65	0.07	0.06
10	assign (segid 3A4 and resid 37 and name N) (segid 3A4 and resid 39 and name CA)	5.34	0.07	0.07
	assign (segid 3A4 and resid 37 and name N) (segid 3A4 and resid 39 and name CB)	5.42	0.09	0.08
	assign (segid 3A4 and resid 37 and name N) (segid 3A4 and resid 39 and name N)	4.32	0.04	0.05
	assign (segid 3A4 and resid 37 and name N) (segid 3A4 and resid 39 and name O)	6.85	0.07	0.07
	assign (segid 3A4 and resid 37 and name N) (segid 3A4 and resid 40 and name C)	6.56	0.11	0.11
15	assign (segid 3A4 and resid 37 and name N) (segid 3A4 and resid 40 and name CA)	5.74	0.08	0.08
	assign (segid 3A4 and resid 37 and name N) (segid 3A4 and resid 40 and name CB)	5.27	0.12	0.11
	assign (segid 3A4 and resid 37 and name N) (segid 3A4 and resid 40 and name N)	4.90	0.08	0.08
	assign (segid 3A4 and resid 37 and name N) (segid 3A4 and resid 40 and name O)	7.76	0.10	0.10
20	assign (segid 3A4 and resid 37 and name N) (segid 3A4 and resid 41 and name CA)	7.23	0.21	0.21
	assign (segid 3A4 and resid 37 and name N) (segid 3A4 and resid 41 and name CB)	6.95	0.27	0.27
	assign (segid 3A4 and resid 37 and name N) (segid 3A4 and resid 41 and name N)	6.14	0.17	0.18
	assign (segid 3A4 and resid 37 and name N) (segid 3A4 and resid 41 and name O)	3.32	0.06	0.06
	assign (segid 3A4 and resid 37 and name O) (segid 3A4 and resid 37 and name C)	3.13	0.12	0.13
	assign (segid 3A4 and resid 37 and name O) (segid 3A4 and resid 38 and name CA)	2.77	0.04	0.04
25	assign (segid 3A4 and resid 37 and name O) (segid 3A4 and resid 38 and name CB)	4.21	0.06	0.06
	assign (segid 3A4 and resid 37 and name O) (segid 3A4 and resid 38 and name N)	2.24	0.01	0.01
	assign (segid 3A4 and resid 37 and name O) (segid 3A4 and resid 38 and name O)	3.68	0.16	0.16
	assign (segid 3A4 and resid 37 and name O) (segid 3A4 and resid 39 and name C)	4.37	0.22	0.22
	assign (segid 3A4 and resid 37 and name O) (segid 3A4 and resid 39 and name CA)	4.62	0.22	0.22
30	assign (segid 3A4 and resid 37 and name O) (segid 3A4 and resid 39 and name CB)	5.61	0.20	0.21
	assign (segid 3A4 and resid 37 and name O) (segid 3A4 and resid 39 and name N)	3.61	0.18	0.18
	assign (segid 3A4 and resid 37 and name O) (segid 3A4 and resid 39 and name O)	5.24	0.24	0.24
	assign (segid 3A4 and resid 37 and name O) (segid 3A4 and resid 40 and name C)	4.15	0.30	0.29
35	assign (segid 3A4 and resid 37 and name O) (segid 3A4 and resid 40 and name CA)	4.13	0.24	0.25
	assign (segid 3A4 and resid 37 and name O) (segid 3A4 and resid 40 and name CB)	3.99	0.24	0.24
	assign (segid 3A4 and resid 37 and name O) (segid 3A4 and resid 40 and name N)	3.66	0.21	0.21
	assign (segid 3A4 and resid 37 and name O) (segid 3A4 and resid 40 and name O)	5.29	0.29	0.29
	assign (segid 3A4 and resid 37 and name O) (segid 3A4 and resid 41 and name C)	5.20	0.37	0.37
	assign (segid 3A4 and resid 37 and name O) (segid 3A4 and resid 41 and name CA)	4.00	0.36	0.37
40	assign (segid 3A4 and resid 37 and name O) (segid 3A4 and resid 41 and name CB)	3.56	0.37	0.37
	assign (segid 3A4 and resid 37 and name O) (segid 3A4 and resid 41 and name N)	3.26	0.36	0.36
	assign (segid 3A4 and resid 37 and name O) (segid 3A4 and resid 41 and name O)	6.31	0.37	0.36
	assign (segid 3A4 and resid 37 and name O) (segid 3A4 and resid 42 and name CA)	6.63	0.36	0.37
45	assign (segid 3A4 and resid 37 and name O) (segid 3A4 and resid 42 and name CB)	6.86	0.34	0.35
	assign (segid 3A4 and resid 37 and name O) (segid 3A4 and resid 42 and name N)	5.27	0.37	0.37
	assign (segid 3A4 and resid 37 and name O) (segid 3A4 and resid 381 and name O)	1.23	0.00	0.00
	assign (segid 3A4 and resid 381 and name C) (segid 3A4 and resid 382 and name C)	3.49	0.05	0.04
	assign (segid 3A4 and resid 381 and name C) (segid 3A4 and resid 382 and name CB)	2.45	0.02	0.01
50	assign (segid 3A4 and resid 381 and name C) (segid 3A4 and resid 382 and name N)	3.51	0.05	0.05
	assign (segid 3A4 and resid 381 and name C) (segid 3A4 and resid 382 and name O)	1.32	0.02	0.02
	assign (segid 3A4 and resid 381 and name C) (segid 3A4 and resid 382 and name O)	4.63	0.02	0.02
	assign (segid 3A4 and resid 381 and name C) (segid 3A4 and resid 383 and name C)	5.90	0.18	0.17
	assign (segid 3A4 and resid 381 and name C) (segid 3A4 and resid 383 and name CA)	4.96	0.15	0.16
55	assign (segid 3A4 and resid 381 and name C) (segid 3A4 and resid 383 and name N)	3.57	0.14	0.14
	assign (segid 3A4 and resid 381 and name C) (segid 3A4 and resid 383 and name O)	7.06	0.17	0.17
	assign (segid 3A4 and resid 381 and name C) (segid 3A4 and resid 384 and name C)	7.10	0.24	0.25
	assign (segid 3A4 and resid 381 and name C) (segid 3A4 and resid 384 and name CB)	6.86	0.24	0.23
	assign (segid 3A4 and resid 381 and name C) (segid 3A4 and resid 384 and name N)	7.18	0.28	0.29
60	assign (segid 3A4 and resid 381 and name C) (segid 3A4 and resid 384 and name O)	5.66	0.22	0.21
	assign (segid 3A4 and resid 381 and name C) (segid 3A4 and resid 385 and name C)	6.72	0.29	0.30
	assign (segid 3A4 and resid 381 and name C) (segid 3A4 and resid 385 and name CA)	7.11	0.25	0.25
	assign (segid 3A4 and resid 381 and name C) (segid 3A4 and resid 385 and name N)	6.47	0.24	0.24
	assign (segid 3A4 and resid 381 and name C) (segid 3A4 and resid 385 and name O)	5.75	0.33	0.32
65	assign (segid 3A4 and resid 381 and name C) (segid 3A4 and resid 381 and name O)	1.53	0.01	0.01
	assign (segid 3A4 and resid 381 and name CA) (segid 3A4 and resid 381 and name O)	2.39	0.02	0.02
	assign (segid 3A4 and resid 381 and name CA) (segid 3A4 and resid 382 and name C)	4.74	0.07	0.07
	assign (segid 3A4 and resid 381 and name CA) (segid 3A4 and resid 382 and name CA)	3.82	0.01	0.01
	assign (segid 3A4 and resid 381 and name CA) (segid 3A4 and resid 382 and name CB)	4.72	0.04	0.04
70	assign (segid 3A4 and resid 381 and name CA) (segid 3A4 and resid 382 and name N)	2.43	0.02	0.02
	assign (segid 3A4 and resid 381 and name CA) (segid 3A4 and resid 382 and name O)	5.89	0.07	0.06
	assign (segid 3A4 and resid 381 and name CA) (segid 3A4 and resid 383 and name C)	6.99	0.20	0.20
	assign (segid 3A4 and resid 381 and name CA) (segid 3A4 and resid 383 and name CA)	5.87	0.21	0.21
	assign (segid 3A4 and resid 381 and name CA) (segid 3A4 and resid 383 and name N)	4.60	0.18	0.19
75	assign (segid 3A4 and resid 381 and name CA) (segid 3A4 and resid 384 and name CA)	8.14	0.24	0.24
	assign (segid 3A4 and resid 381 and name CA) (segid 3A4 and resid 384 and name CB)	8.40	0.30	0.30
	assign (segid 3A4 and resid 381 and name CA) (segid 3A4 and resid 384 and name N)	6.88	0.23	0.22
	assign (segid 3A4 and resid 381 and name CA) (segid 3A4 and resid 385 and name CA)	8.59	0.24	0.24
	assign (segid 3A4 and resid 381 and name CA) (segid 3A4 and resid 385 and name O)	7.25	0.33	0.33
80	assign (segid 3A4 and resid 381 and name CA) (segid 3A4 and resid 386 and name CA)	9.35	0.31	0.31
	assign (segid 3A4 and resid 381 and name CA) (segid 3A4 and resid 387 and name CA)	12.79	0.23	0.22
	assign (segid 3A4 and resid 381 and name CA) (segid 3A4 and resid 388 and name CA)	15.90	0.23	0.22
	assign (segid 3A4 and resid 381 and name CA) (segid 3A4 and resid 388 and name CB)	17.25	0.20	0.19

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	assign (segid 3A4 and resid 382 and name CA)	(segid 3A4 and resid 384 and name C)	5.39	0.07	0.06
	assign (segid 3A4 and resid 382 and name CA)	(segid 3A4 and resid 384 and name CA)	5.45	0.05	0.05
	assign (segid 3A4 and resid 382 and name CA)	(segid 3A4 and resid 384 and name CB)	6.19	0.08	0.09
	assign (segid 3A4 and resid 382 and name CA)	(segid 3A4 and resid 384 and name CG)	7.00	0.11	0.11
5	assign (segid 3A4 and resid 382 and name CA)	(segid 3A4 and resid 384 and name N)	4.33	0.05	0.04
	assign (segid 3A4 and resid 382 and name CA)	(segid 3A4 and resid 384 and name O)	6.42	0.08	0.08
	assign (segid 3A4 and resid 382 and name CA)	(segid 3A4 and resid 385 and name C)	4.83	0.19	0.19
	assign (segid 3A4 and resid 382 and name CA)	(segid 3A4 and resid 385 and name CA)	4.98	0.17	0.16
	assign (segid 3A4 and resid 382 and name CA)	(segid 3A4 and resid 385 and name N)	4.48	0.10	0.10
	assign (segid 3A4 and resid 382 and name CA)	(segid 3A4 and resid 385 and name O)	4.13	0.19	0.19
10	assign (segid 3A4 and resid 382 and name CA)	(segid 3A4 and resid 386 and name CA)	6.36	0.22	0.23
	assign (segid 3A4 and resid 382 and name CA)	(segid 3A4 and resid 386 and name N)	5.91	0.23	0.22
	assign (segid 3A4 and resid 382 and name CA)	(segid 3A4 and resid 387 and name CA)	10.01	0.12	0.12
	assign (segid 3A4 and resid 382 and name CA)	(segid 3A4 and resid 388 and name CA)	12.95	0.14	0.15
	assign (segid 3A4 and resid 382 and name CA)	(segid 3A4 and resid 388 and name CB)	14.26	0.13	0.14
15	assign (segid 3A4 and resid 382 and name CA)	(segid 3A4 and resid 389 and name CA)	11.83	0.27	0.27
	assign (segid 3A4 and resid 382 and name CA)	(segid 3A4 and resid 389 and name CB)	11.98	0.34	0.34
	assign (segid 3A4 and resid 382 and name CA)	(segid 3A4 and resid 390 and name CA)	9.04	0.14	0.14
	assign (segid 3A4 and resid 382 and name CA)	(segid 3A4 and resid 390 and name CB)	8.83	0.24	0.24
20	assign (segid 3A4 and resid 382 and name CA)	(segid 3A4 and resid 391 and name CA)	10.10	0.08	0.08
	assign (segid 3A4 and resid 382 and name CA)	(segid 3A4 and resid 391 and name CB)	9.46	0.10	0.09
	assign (segid 3A4 and resid 382 and name CA)	(segid 3A4 and resid 392 and name CA)	13.54	0.11	0.10
	assign (segid 3A4 and resid 382 and name CA)	(segid 3A4 and resid 392 and name CB)	14.79	0.08	0.07
	assign (segid 3A4 and resid 382 and name CA)	(segid 3A4 and resid 393 and name CA)	14.03	0.12	0.13
	assign (segid 3A4 and resid 382 and name CA)	(segid 3A4 and resid 394 and name CA)	11.32	0.36	0.36
25	assign (segid 3A4 and resid 382 and name CA)	(segid 3A4 and resid 394 and name CB)	10.31	0.40	0.41
	assign (segid 3A4 and resid 382 and name CA)	(segid 3A4 and resid 395 and name CA)	14.31	0.56	0.55
	assign (segid 3A4 and resid 382 and name CA)	(segid 3A4 and resid 396 and name CA)	16.50	0.34	0.34
	assign (segid 3A4 and resid 382 and name CA)	(segid 3A4 and resid 396 and name CB)	17.12	0.26	0.26
	assign (segid 3A4 and resid 382 and name CA)	(segid 3A4 and resid 397 and name CA)	14.25	0.28	0.28
30	assign (segid 3A4 and resid 382 and name CA)	(segid 3A4 and resid 397 and name CB)	12.94	0.25	0.26
	assign (segid 3A4 and resid 382 and name CA)	(segid 3A4 and resid 398 and name CA)	13.88	0.53	0.52
	assign (segid 3A4 and resid 382 and name CA)	(segid 3A4 and resid 398 and name CB)	13.25	0.58	0.57
	assign (segid 3A4 and resid 382 and name CA)	(segid 3A4 and resid 399 and name CA)	17.60	0.51	0.52
	assign (segid 3A4 and resid 382 and name CA)	(segid 3A4 and resid 399 and name CB)	18.35	0.48	0.48
35	assign (segid 3A4 and resid 382 and name CA)	(segid 3A4 and resid 400 and name CA)	18.67	0.40	0.40
	assign (segid 3A4 and resid 382 and name CA)	(segid 3A4 and resid 400 and name CB)	18.43	0.42	0.41
	assign (segid 3A4 and resid 382 and name CA)	(segid 3A4 and resid 401 and name CA)	16.95	0.43	0.43
	assign (segid 3A4 and resid 382 and name CA)	(segid 3A4 and resid 402 and name CA)	18.41	0.48	0.48
40	assign (segid 3A4 and resid 382 and name CA)	(segid 3A4 and resid 402 and name CB)	18.14	0.54	0.53
	assign (segid 3A4 and resid 382 and name CA)	(segid 3A4 and resid 431 and name CA)	15.86	1.18	1.18
	assign (segid 3A4 and resid 382 and name CA)	(segid 3A4 and resid 432 and name CA)	15.39	0.34	0.34
	assign (segid 3A4 and resid 382 and name CA)	(segid 3A4 and resid 434 and name CA)	17.37	0.84	0.84
	assign (segid 3A4 and resid 382 and name CA)	(segid 3A4 and resid 434 and name CB)	7.34	0.25	0.25
	assign (segid 3A4 and resid 382 and name CA)	(segid 3A4 and resid 383 and name C)	5.47	0.06	0.05
45	assign (segid 3A4 and resid 382 and name CB)	(segid 3A4 and resid 383 and name CA)	4.88	0.05	0.05
	assign (segid 3A4 and resid 382 and name CB)	(segid 3A4 and resid 383 and name N)	3.71	0.06	0.06
	assign (segid 3A4 and resid 382 and name CB)	(segid 3A4 and resid 383 and name O)	6.33	0.08	0.08
	assign (segid 3A4 and resid 382 and name CB)	(segid 3A4 and resid 384 and name C)	6.00	0.14	0.13
	assign (segid 3A4 and resid 382 and name CB)	(segid 3A4 and resid 384 and name CA)	6.37	0.12	0.12
50	assign (segid 3A4 and resid 382 and name CB)	(segid 3A4 and resid 384 and name CB)	7.26	0.16	0.16
	assign (segid 3A4 and resid 382 and name CB)	(segid 3A4 and resid 384 and name N)	5.40	0.10	0.09
	assign (segid 3A4 and resid 382 and name CB)	(segid 3A4 and resid 384 and name O)	6.95	0.17	0.16
	assign (segid 3A4 and resid 382 and name CB)	(segid 3A4 and resid 385 and name C)	4.74	0.23	0.22
	assign (segid 3A4 and resid 382 and name CB)	(segid 3A4 and resid 385 and name CA)	4.94	0.17	0.18
55	assign (segid 3A4 and resid 382 and name CB)	(segid 3A4 and resid 385 and name N)	4.87	0.13	0.12
	assign (segid 3A4 and resid 382 and name CB)	(segid 3A4 and resid 385 and name O)	4.27	0.26	0.26
	assign (segid 3A4 and resid 382 and name CB)	(segid 3A4 and resid 386 and name C)	7.36	0.30	0.30
	assign (segid 3A4 and resid 382 and name CB)	(segid 3A4 and resid 386 and name CA)	5.98	0.31	0.31
	assign (segid 3A4 and resid 382 and name CB)	(segid 3A4 and resid 386 and name N)	5.58	0.27	0.27
60	assign (segid 3A4 and resid 382 and name CB)	(segid 3A4 and resid 387 and name CA)	9.56	0.31	0.32
	assign (segid 3A4 and resid 382 and name CB)	(segid 3A4 and resid 388 and name CA)	12.66	0.29	0.29
	assign (segid 3A4 and resid 382 and name CB)	(segid 3A4 and resid 388 and name CB)	13.88	0.26	0.27
	assign (segid 3A4 and resid 382 and name CB)	(segid 3A4 and resid 389 and name CA)	11.62	0.31	0.31
	assign (segid 3A4 and resid 382 and name CB)	(segid 3A4 and resid 389 and name CB)	11.63	0.34	0.35
65	assign (segid 3A4 and resid 382 and name CB)	(segid 3A4 and resid 390 and name CA)	9.23	0.26	0.26
	assign (segid 3A4 and resid 382 and name CB)	(segid 3A4 and resid 390 and name CB)	9.10	0.37	0.36
	assign (segid 3A4 and resid 382 and name CB)	(segid 3A4 and resid 391 and name CA)	10.70	0.15	0.15
	assign (segid 3A4 and resid 382 and name CB)	(segid 3A4 and resid 391 and name CB)	10.21	0.15	0.14
	assign (segid 3A4 and resid 382 and name CB)	(segid 3A4 and resid 392 and name CA)	14.22	0.21	0.20
70	assign (segid 3A4 and resid 382 and name CB)	(segid 3A4 and resid 392 and name CB)	15.38	0.17	0.17
	assign (segid 3A4 and resid 382 and name CB)	(segid 3A4 and resid 393 and name CA)	14.99	0.18	0.18
	assign (segid 3A4 and resid 382 and name CB)	(segid 3A4 and resid 394 and name CA)	12.49	0.39	0.40
	assign (segid 3A4 and resid 382 and name CB)	(segid 3A4 and resid 394 and name CB)	11.47	0.46	0.45
	assign (segid 3A4 and resid 382 and name CB)	(segid 3A4 and resid 395 and name CA)	15.57	0.58	0.59
75	assign (segid 3A4 and resid 382 and name CB)	(segid 3A4 and resid 396 and name CA)	17.76	0.33	0.33
	assign (segid 3A4 and resid 382 and name CB)	(segid 3A4 and resid 396 and name CB)	18.30	0.27	0.27
	assign (segid 3A4 and resid 382 and name CB)	(segid 3A4 and resid 397 and name CA)	15.55	0.25	0.26
	assign (segid 3A4 and resid 382 and name CB)	(segid 3A4 and resid 397 and name CB)	14.21	0.23	0.23
	assign (segid 3A4 and resid 382 and name CB)	(segid 3A4 and resid 398 and name CA)	15.34	0.51	0.52
80	assign (segid 3A4 and resid 382 and name CB)	(segid 3A4 and resid 398 and name CB)	14.72	0.58	0.57
	assign (segid 3A4 and resid 382 and name CB)	(segid 3A4 and resid 399 and name CA)	19.05	0.51	0.51
	assign (segid 3A4 and resid 382 and name CB)	(segid 3A4 and resid 401 and name CA)	18.39	0.41	0.41

	assign (segid 3A4 and resid 382 and name CB)	(segid 3A4 and resid 431 and name CA)	15.70	1.22	1.22
	assign (segid 3A4 and resid 382 and name CB)	(segid 3A4 and resid 433 and name CA)	15.69	0.41	0.40
	assign (segid 3A4 and resid 382 and name CB)	(segid 3A4 and resid 434 and name CA)	17.91	0.91	0.90
	assign (segid 3A4 and resid 382 and name N)	(segid 3A4 and resid 382 and name C)	2.49	0.05	0.05
5	assign (segid 3A4 and resid 382 and name N)	(segid 3A4 and resid 382 and name CA)	1.47	0.02	0.02
	assign (segid 3A4 and resid 382 and name N)	(segid 3A4 and resid 382 and name CB)	2.47	0.04	0.04
	assign (segid 3A4 and resid 382 and name N)	(segid 3A4 and resid 382 and name O)	3.55	0.07	0.06
	assign (segid 3A4 and resid 382 and name N)	(segid 3A4 and resid 383 and name C)	5.24	0.09	0.09
	assign (segid 3A4 and resid 382 and name N)	(segid 3A4 and resid 383 and name CA)	4.24	0.10	0.10
10	assign (segid 3A4 and resid 382 and name N)	(segid 3A4 and resid 383 and name N)	2.84	0.11	0.11
	assign (segid 3A4 and resid 382 and name N)	(segid 3A4 and resid 383 and name O)	6.32	0.11	0.11
	assign (segid 3A4 and resid 382 and name N)	(segid 3A4 and resid 384 and name C)	6.61	0.11	0.11
	assign (segid 3A4 and resid 382 and name N)	(segid 3A4 and resid 384 and name CA)	6.46	0.09	0.08
	assign (segid 3A4 and resid 382 and name N)	(segid 3A4 and resid 384 and name CB)	7.05	0.11	0.11
15	assign (segid 3A4 and resid 382 and name N)	(segid 3A4 and resid 384 and name CG)	7.65	0.10	0.09
	assign (segid 3A4 and resid 382 and name N)	(segid 3A4 and resid 384 and name N)	5.20	0.08	0.08
	assign (segid 3A4 and resid 382 and name N)	(segid 3A4 and resid 384 and name O)	7.68	0.12	0.11
	assign (segid 3A4 and resid 382 and name N)	(segid 3A4 and resid 385 and name C)	6.21	0.21	0.22
	assign (segid 3A4 and resid 382 and name N)	(segid 3A4 and resid 385 and name CA)	6.41	0.18	0.18
20	assign (segid 3A4 and resid 382 and name N)	(segid 3A4 and resid 385 and name N)	5.82	0.13	0.14
	assign (segid 3A4 and resid 382 and name N)	(segid 3A4 and resid 385 and name O)	5.41	0.23	0.22
	assign (segid 3A4 and resid 382 and name N)	(segid 3A4 and resid 386 and name N)	7.27	0.25	0.24
	assign (segid 3A4 and resid 382 and name O)	(segid 3A4 and resid 382 and name CB)	2.74	0.05	0.04
	assign (segid 3A4 and resid 382 and name O)	(segid 3A4 and resid 383 and name C)	2.99	0.06	0.06
25	assign (segid 3A4 and resid 382 and name O)	(segid 3A4 and resid 383 and name CA)	2.71	0.05	0.05
	assign (segid 3A4 and resid 382 and name O)	(segid 3A4 and resid 383 and name N)	2.24	0.02	0.02
	assign (segid 3A4 and resid 382 and name O)	(segid 3A4 and resid 383 and name O)	3.66	0.08	0.09
	assign (segid 3A4 and resid 382 and name O)	(segid 3A4 and resid 384 and name C)	4.15	0.09	0.10
	assign (segid 3A4 and resid 382 and name O)	(segid 3A4 and resid 384 and name CA)	4.29	0.06	0.05
30	assign (segid 3A4 and resid 382 and name O)	(segid 3A4 and resid 384 and name CB)	5.50	0.07	0.07
	assign (segid 3A4 and resid 382 and name O)	(segid 3A4 and resid 384 and name CD1)	6.73	0.26	0.26
	assign (segid 3A4 and resid 382 and name O)	(segid 3A4 and resid 384 and name CD2)	7.07	0.29	0.28
	assign (segid 3A4 and resid 382 and name O)	(segid 3A4 and resid 384 and name CG)	6.34	0.09	0.09
35	assign (segid 3A4 and resid 382 and name O)	(segid 3A4 and resid 384 and name N)	3.26	0.06	0.07
	assign (segid 3A4 and resid 382 and name O)	(segid 3A4 and resid 384 and name O)	5.29	0.11	0.10
	assign (segid 3A4 and resid 382 and name O)	(segid 3A4 and resid 385 and name C)	4.35	0.21	0.22
	assign (segid 3A4 and resid 382 and name O)	(segid 3A4 and resid 385 and name CA)	3.76	0.19	0.19
	assign (segid 3A4 and resid 382 and name O)	(segid 3A4 and resid 385 and name N)	3.12	0.14	0.14
40	assign (segid 3A4 and resid 382 and name O)	(segid 3A4 and resid 385 and name O)	4.20	0.21	0.20
	assign (segid 3A4 and resid 382 and name O)	(segid 3A4 and resid 386 and name CA)	6.47	0.22	0.21
	assign (segid 3A4 and resid 382 and name O)	(segid 3A4 and resid 386 and name N)	5.52	0.23	0.22
	assign (segid 3A4 and resid 382 and name O)	(segid HEM and resid 1 and name C2A)	7.19	0.34	0.34
	assign (segid 3A4 and resid 382 and name O)	(segid HEM and resid 1 and name C3A)	6.29	0.29	0.29
45	assign (segid 3A4 and resid 382 and name O)	(segid HEM and resid 1 and name C4A)	6.99	0.24	0.23
	assign (segid 3A4 and resid 382 and name O)	(segid HEM and resid 1 and name CHB)	6.78	0.20	0.20
	assign (segid 3A4 and resid 382 and name O)	(segid HEM and resid 1 and name CMA)	5.10	0.27	0.28
	assign (segid 3A4 and resid 382 and name O)	(segid HEM and resid 1 and name CMB)	7.13	0.14	0.14
	assign (segid 3A4 and resid 383 and name C)	(segid 3A4 and resid 383 and name O)	1.22	0.00	0.01
	assign (segid 3A4 and resid 383 and name C)	(segid 3A4 and resid 384 and name C)	3.36	0.06	0.05
50	assign (segid 3A4 and resid 383 and name C)	(segid 3A4 and resid 384 and name CA)	2.44	0.02	0.01
	assign (segid 3A4 and resid 383 and name C)	(segid 3A4 and resid 384 and name CB)	3.60	0.05	0.04
	assign (segid 3A4 and resid 383 and name C)	(segid 3A4 and resid 384 and name CD1)	4.20	0.14	0.14
	assign (segid 3A4 and resid 383 and name C)	(segid 3A4 and resid 384 and name CD2)	4.59	0.21	0.20
	assign (segid 3A4 and resid 383 and name C)	(segid 3A4 and resid 384 and name CG)	3.91	0.11	0.11
55	assign (segid 3A4 and resid 383 and name C)	(segid 3A4 and resid 384 and name N)	1.33	0.00	0.00
	assign (segid 3A4 and resid 383 and name C)	(segid 3A4 and resid 384 and name O)	4.51	0.05	0.06
	assign (segid 3A4 and resid 383 and name C)	(segid 3A4 and resid 385 and name C)	5.56	0.14	0.13
	assign (segid 3A4 and resid 383 and name C)	(segid 3A4 and resid 385 and name CA)	4.68	0.11	0.11
	assign (segid 3A4 and resid 383 and name C)	(segid 3A4 and resid 385 and name N)	3.31	0.11	0.11
60	assign (segid 3A4 and resid 383 and name C)	(segid 3A4 and resid 385 and name O)	5.36	0.15	0.15
	assign (segid 3A4 and resid 383 and name C)	(segid 3A4 and resid 386 and name N)	6.85	0.12	0.12
	assign (segid 3A4 and resid 383 and name C)	(segid 3A4 and resid 391 and name CA)	7.45	0.09	0.08
	assign (segid 3A4 and resid 383 and name C)	(segid 3A4 and resid 391 and name CB)	6.35	0.10	0.10
	assign (segid 3A4 and resid 383 and name C)	(segid 3A4 and resid 391 and name N)	7.12	0.08	0.08
65	assign (segid 3A4 and resid 383 and name C)	(segid HEM and resid 1 and name C1A)	6.94	0.14	0.14
	assign (segid 3A4 and resid 383 and name C)	(segid HEM and resid 1 and name C1B)	5.25	0.11	0.12
	assign (segid 3A4 and resid 383 and name C)	(segid HEM and resid 1 and name C2A)	6.25	0.15	0.16
	assign (segid 3A4 and resid 383 and name C)	(segid HEM and resid 1 and name C2B)	5.18	0.12	0.12
	assign (segid 3A4 and resid 383 and name C)	(segid HEM and resid 1 and name C3A)	5.10	0.12	0.13
70	assign (segid 3A4 and resid 383 and name C)	(segid HEM and resid 1 and name C3B)	6.37	0.14	0.14
	assign (segid 3A4 and resid 383 and name C)	(segid HEM and resid 1 and name C4A)	5.20	0.12	0.11
	assign (segid 3A4 and resid 383 and name C)	(segid HEM and resid 1 and name C4B)	7.04	0.12	0.12
	assign (segid 3A4 and resid 383 and name C)	(segid HEM and resid 1 and name CAA)	7.00	0.20	0.21
	assign (segid 3A4 and resid 383 and name C)	(segid HEM and resid 1 and name CAB)	7.18	0.15	0.15
75	assign (segid 3A4 and resid 383 and name C)	(segid HEM and resid 1 and name CBB)	7.21	0.25	0.25
	assign (segid 3A4 and resid 383 and name C)	(segid HEM and resid 1 and name CHB)	4.56	0.10	0.10
	assign (segid 3A4 and resid 383 and name C)	(segid HEM and resid 1 and name CNA)	4.36	0.09	0.08
	assign (segid 3A4 and resid 383 and name C)	(segid HEM and resid 1 and name CNB)	4.37	0.09	0.10
	assign (segid 3A4 and resid 383 and name C)	(segid HEM and resid 1 and name FE)	7.54	0.17	0.16
80	assign (segid 3A4 and resid 383 and name C)	(segid HEM and resid 1 and name NA)	6.39	0.12	0.12
	assign (segid 3A4 and resid 383 and name C)	(segid HEM and resid 1 and name NB)	6.46	0.12	0.11
	assign (segid 3A4 and resid 383 and name CA)	(segid 3A4 and resid 383 and name C)	1.53	0.01	0.00
	assign (segid 3A4 and resid 383 and name CA)	(segid 3A4 and resid 383 and name O)	2.38	0.02	0.03

	assign (segid 3A4 and resid 383 and name CA)	(segid 3A4 and resid 384 and name C)	4.63	0.06	0.06
	assign (segid 3A4 and resid 383 and name CA)	(segid 3A4 and resid 384 and name CA)	3.82	0.01	0.01
	assign (segid 3A4 and resid 383 and name CA)	(segid 3A4 and resid 384 and name CB)	4.79	0.03	0.04
	assign (segid 3A4 and resid 383 and name CA)	(segid 3A4 and resid 384 and name CD1)	5.13	0.31	0.32
	assign (segid 3A4 and resid 383 and name CA)	(segid 3A4 and resid 384 and name CD2)	5.54	0.35	0.34
5	assign (segid 3A4 and resid 383 and name CA)	(segid 3A4 and resid 384 and name CG)	4.98	0.10	0.11
	assign (segid 3A4 and resid 383 and name CA)	(segid 3A4 and resid 384 and name N)	2.44	0.01	0.01
	assign (segid 3A4 and resid 383 and name CA)	(segid 3A4 and resid 384 and name O)	5.83	0.06	0.06
	assign (segid 3A4 and resid 383 and name CA)	(segid 3A4 and resid 385 and name C)	6.25	0.16	0.16
	assign (segid 3A4 and resid 383 and name CA)	(segid 3A4 and resid 385 and name CA)	5.54	0.15	0.14
10	assign (segid 3A4 and resid 383 and name CA)	(segid 3A4 and resid 385 and name N)	4.30	0.11	0.12
	assign (segid 3A4 and resid 383 and name CA)	(segid 3A4 and resid 385 and name O)	5.89	0.16	0.17
	assign (segid 3A4 and resid 383 and name CA)	(segid 3A4 and resid 386 and name CA)	8.52	0.16	0.15
	assign (segid 3A4 and resid 383 and name CA)	(segid 3A4 and resid 386 and name N)	7.55	0.16	0.15
	assign (segid 3A4 and resid 383 and name CA)	(segid 3A4 and resid 387 and name CA)	12.04	0.20	0.20
15	assign (segid 3A4 and resid 383 and name CA)	(segid 3A4 and resid 388 and name CA)	14.26	0.10	0.10
	assign (segid 3A4 and resid 383 and name CA)	(segid 3A4 and resid 388 and name CB)	15.62	0.11	0.11
	assign (segid 3A4 and resid 383 and name CA)	(segid 3A4 and resid 389 and name CA)	12.27	0.22	0.23
	assign (segid 3A4 and resid 383 and name CA)	(segid 3A4 and resid 389 and name CB)	12.38	0.33	0.33
	assign (segid 3A4 and resid 383 and name CA)	(segid 3A4 and resid 390 and name CA)	9.34	0.11	0.11
20	assign (segid 3A4 and resid 383 and name CA)	(segid 3A4 and resid 390 and name CB)	9.51	0.26	0.25
	assign (segid 3A4 and resid 383 and name CA)	(segid 3A4 and resid 391 and name CA)	8.92	0.07	0.08
	assign (segid 3A4 and resid 383 and name CA)	(segid 3A4 and resid 391 and name CB)	7.84	0.09	0.09
	assign (segid 3A4 and resid 383 and name CA)	(segid 3A4 and resid 392 and name CA)	12.37	0.06	0.06
	assign (segid 3A4 and resid 383 and name CA)	(segid 3A4 and resid 392 and name CB)	13.60	0.09	0.08
25	assign (segid 3A4 and resid 383 and name CA)	(segid 3A4 and resid 393 and name CA)	12.00	0.07	0.08
	assign (segid 3A4 and resid 383 and name CA)	(segid 3A4 and resid 394 and name CA)	9.49	0.20	0.20
	assign (segid 3A4 and resid 383 and name CA)	(segid 3A4 and resid 394 and name CB)	8.93	0.27	0.26
	assign (segid 3A4 and resid 383 and name CA)	(segid 3A4 and resid 395 and name CA)	12.71	0.33	0.33
	assign (segid 3A4 and resid 383 and name CA)	(segid 3A4 and resid 396 and name CA)	14.19	0.17	0.17
30	assign (segid 3A4 and resid 383 and name CA)	(segid 3A4 and resid 396 and name CB)	14.75	0.24	0.24
	assign (segid 3A4 and resid 383 and name CA)	(segid 3A4 and resid 397 and name CA)	11.41	0.17	0.17
	assign (segid 3A4 and resid 383 and name CA)	(segid 3A4 and resid 397 and name CB)	10.04	0.18	0.18
	assign (segid 3A4 and resid 383 and name CA)	(segid 3A4 and resid 398 and name CA)	11.51	0.32	0.31
	assign (segid 3A4 and resid 383 and name CA)	(segid 3A4 and resid 398 and name CB)	11.23	0.37	0.36
35	assign (segid 3A4 and resid 383 and name CA)	(segid 3A4 and resid 399 and name CA)	15.26	0.30	0.30
	assign (segid 3A4 and resid 383 and name CA)	(segid 3A4 and resid 399 and name CB)	16.09	0.26	0.27
	assign (segid 3A4 and resid 383 and name CA)	(segid 3A4 and resid 400 and name CA)	15.73	0.30	0.31
	assign (segid 3A4 and resid 383 and name CA)	(segid 3A4 and resid 400 and name CB)	15.35	0.36	0.37
40	assign (segid 3A4 and resid 383 and name CA)	(segid 3A4 and resid 401 and name CA)	13.94	0.31	0.31
	assign (segid 3A4 and resid 383 and name CA)	(segid 3A4 and resid 402 and name CA)	15.92	0.30	0.30
	assign (segid 3A4 and resid 383 and name CA)	(segid 3A4 and resid 402 and name CB)	15.88	0.32	0.33
	assign (segid 3A4 and resid 383 and name CA)	(segid 3A4 and resid 403 and name CA)	19.06	0.31	0.31
	assign (segid 3A4 and resid 383 and name CA)	(segid 3A4 and resid 403 and name CB)	19.41	0.31	0.30
45	assign (segid 3A4 and resid 383 and name CA)	(segid 3A4 and resid 404 and name CA)	19.00	0.32	0.32
	assign (segid 3A4 and resid 383 and name CA)	(segid 3A4 and resid 404 and name CB)	18.07	0.37	0.38
	assign (segid 3A4 and resid 383 and name CA)	(segid 3A4 and resid 405 and name CA)	18.47	0.32	0.32
	assign (segid 3A4 and resid 383 and name CA)	(segid 3A4 and resid 405 and name CB)	17.27	0.36	0.36
	assign (segid 3A4 and resid 383 and name CA)	(segid 3A4 and resid 427 and name CA)	17.60	0.32	0.32
50	assign (segid 3A4 and resid 383 and name CA)	(segid 3A4 and resid 429 and name CA)	16.64	0.92	0.93
	assign (segid 3A4 and resid 383 and name CA)	(segid 3A4 and resid 430 and name CA)	15.74	1.40	1.40
	assign (segid 3A4 and resid 383 and name CA)	(segid 3A4 and resid 431 and name CA)	13.48	1.07	1.07
	assign (segid 3A4 and resid 383 and name CA)	(segid 3A4 and resid 433 and name CA)	12.31	0.25	0.25
	assign (segid 3A4 and resid 383 and name CA)	(segid 3A4 and resid 434 and name CA)	13.98	0.77	0.76
55	assign (segid 3A4 and resid 383 and name CA)	(segid 3A4 and resid 435 and name CA)	16.80	0.61	0.62
	assign (segid 3A4 and resid 383 and name CA)	(segid HEM and resid 1 and name C1B)	6.53	0.12	0.12
	assign (segid 3A4 and resid 383 and name CA)	(segid HEM and resid 1 and name C2A)	7.62	0.18	0.19
	assign (segid 3A4 and resid 383 and name CA)	(segid HEM and resid 1 and name C2B)	6.24	0.11	0.11
	assign (segid 3A4 and resid 383 and name CA)	(segid HEM and resid 1 and name C3A)	6.46	0.17	0.16
	assign (segid 3A4 and resid 383 and name CA)	(segid HEM and resid 1 and name C3B)	7.41	0.13	0.13
60	assign (segid 3A4 and resid 383 and name CA)	(segid HEM and resid 1 and name C4A)	6.61	0.13	0.14
	assign (segid 3A4 and resid 383 and name CA)	(segid HEM and resid 1 and name CHB)	5.91	0.13	0.12
	assign (segid 3A4 and resid 383 and name CA)	(segid HEM and resid 1 and name CMA)	5.51	0.14	0.15
	assign (segid 3A4 and resid 383 and name CA)	(segid HEM and resid 1 and name CMB)	5.16	0.09	0.09
	assign (segid 3A4 and resid 383 and name CA)	(segid HEM and resid 1 and name NB)	7.79	0.11	0.11
65	assign (segid 3A4 and resid 383 and name N)	(segid 3A4 and resid 383 and name C)	2.49	0.02	0.02
	assign (segid 3A4 and resid 383 and name N)	(segid 3A4 and resid 383 and name CA)	1.46	0.01	0.00
	assign (segid 3A4 and resid 383 and name N)	(segid 3A4 and resid 383 and name O)	3.57	0.03	0.04
	assign (segid 3A4 and resid 383 and name N)	(segid 3A4 and resid 384 and name C)	4.76	0.05	0.06
70	assign (segid 3A4 and resid 383 and name N)	(segid 3A4 and resid 384 and name CA)	4.21	0.03	0.02
	assign (segid 3A4 and resid 383 and name N)	(segid 3A4 and resid 384 and name CB)	5.03	0.07	0.06
	assign (segid 3A4 and resid 383 and name N)	(segid 3A4 and resid 384 and name CD1)	5.66	0.47	0.48
	assign (segid 3A4 and resid 383 and name N)	(segid 3A4 and resid 384 and name CD2)	6.01	0.49	0.49
	assign (segid 3A4 and resid 383 and name N)	(segid 3A4 and resid 384 and name CG)	5.43	0.11	0.12
	assign (segid 3A4 and resid 383 and name N)	(segid 3A4 and resid 384 and name N)	2.78	0.03	0.03
75	assign (segid 3A4 and resid 383 and name N)	(segid 3A4 and resid 384 and name O)	5.96	0.07	0.06
	assign (segid 3A4 and resid 383 and name N)	(segid 3A4 and resid 385 and name C)	5.70	0.16	0.16
	assign (segid 3A4 and resid 383 and name N)	(segid 3A4 and resid 385 and name CA)	5.32	0.13	0.13
	assign (segid 3A4 and resid 383 and name N)	(segid 3A4 and resid 385 and name N)	4.21	0.10	0.10
80	assign (segid 3A4 and resid 383 and name N)	(segid 3A4 and resid 385 and name O)	5.15	0.17	0.16
	assign (segid 3A4 and resid 383 and name N)	(segid 3A4 and resid 386 and name N)	6.99	0.17	0.17
	assign (segid 3A4 and resid 383 and name N)	(segid HEM and resid 1 and name C1B)	7.71	0.09	0.09
	assign (segid 3A4 and resid 383 and name N)	(segid HEM and resid 1 and name C2B)	7.51	0.08	0.09

	assign (segid 3A4 and resid 383 and name N)	(segid HEM and resid 1 and name C3A)	7.28	0.19	0.20
	assign (segid 3A4 and resid 383 and name N)	(segid HEM and resid 1 and name C4A)	7.57	0.14	0.15
	assign (segid 3A4 and resid 383 and name N)	(segid HEM and resid 1 and name CHB)	7.03	0.12	0.11
	assign (segid 3A4 and resid 383 and name N)	(segid HEM and resid 1 and name CMA)	6.31	0.18	0.18
	assign (segid 3A4 and resid 383 and name N)	(segid HEM and resid 1 and name CHB)	6.52	0.05	0.06
5	assign (segid 3A4 and resid 383 and name N)	(segid HEM and resid 1 and name C)	3.62	0.06	0.06
	assign (segid 3A4 and resid 383 and name O)	(segid 3A4 and resid 384 and name CA)	2.78	0.03	0.03
	assign (segid 3A4 and resid 383 and name O)	(segid 3A4 and resid 384 and name CB)	4.05	0.07	0.07
	assign (segid 3A4 and resid 383 and name O)	(segid 3A4 and resid 384 and name CD1)	4.47	0.28	0.28
	assign (segid 3A4 and resid 383 and name O)	(segid 3A4 and resid 384 and name CD2)	4.89	0.17	0.17
10	assign (segid 3A4 and resid 383 and name O)	(segid 3A4 and resid 384 and name CG)	4.26	0.14	0.15
	assign (segid 3A4 and resid 383 and name O)	(segid 3A4 and resid 384 and name N)	2.25	0.01	0.00
	assign (segid 3A4 and resid 383 and name O)	(segid 3A4 and resid 384 and name O)	4.66	0.07	0.06
	assign (segid 3A4 and resid 383 and name O)	(segid 3A4 and resid 385 and name C)	6.08	0.13	0.13
	assign (segid 3A4 and resid 383 and name O)	(segid 3A4 and resid 385 and name CA)	4.96	0.11	0.11
15	assign (segid 3A4 and resid 383 and name O)	(segid 3A4 and resid 385 and name N)	3.69	0.11	0.11
	assign (segid 3A4 and resid 383 and name O)	(segid 3A4 and resid 385 and name O)	6.10	0.15	0.14
	assign (segid 3A4 and resid 383 and name O)	(segid 3A4 and resid 386 and name N)	7.29	0.11	0.11
	assign (segid 3A4 and resid 383 and name O)	(segid 3A4 and resid 391 and name CA)	7.24	0.14	0.14
20	assign (segid 3A4 and resid 383 and name O)	(segid 3A4 and resid 391 and name CB)	6.10	0.14	0.15
	assign (segid 3A4 and resid 383 and name O)	(segid 3A4 and resid 391 and name N)	7.07	0.12	0.11
	assign (segid 3A4 and resid 383 and name O)	(segid HEM and resid 1 and name C1A)	6.21	0.14	0.13
	assign (segid 3A4 and resid 383 and name O)	(segid HEM and resid 1 and name C1B)	4.34	0.19	0.18
	assign (segid 3A4 and resid 383 and name O)	(segid HEM and resid 1 and name C2A)	5.53	0.12	0.12
25	assign (segid 3A4 and resid 383 and name O)	(segid HEM and resid 1 and name C2B)	4.33	0.19	0.19
	assign (segid 3A4 and resid 383 and name O)	(segid HEM and resid 1 and name C3A)	4.27	0.11	0.12
	assign (segid 3A4 and resid 383 and name O)	(segid HEM and resid 1 and name C3B)	5.61	0.21	0.21
	assign (segid 3A4 and resid 383 and name O)	(segid HEM and resid 1 and name C4A)	4.30	0.13	0.13
	assign (segid 3A4 and resid 383 and name O)	(segid HEM and resid 1 and name C4B)	6.26	0.18	0.19
	assign (segid 3A4 and resid 383 and name O)	(segid HEM and resid 1 and name CAA)	6.40	0.15	0.15
30	assign (segid 3A4 and resid 383 and name O)	(segid HEM and resid 1 and name CAB)	6.52	0.21	0.22
	assign (segid 3A4 and resid 383 and name O)	(segid HEM and resid 1 and name CBA)	6.93	0.34	0.33
	assign (segid 3A4 and resid 383 and name O)	(segid HEM and resid 1 and name CBB)	6.65	0.27	0.28
	assign (segid 3A4 and resid 383 and name O)	(segid HEM and resid 1 and name CHA)	7.57	0.14	0.13
	assign (segid 3A4 and resid 383 and name O)	(segid HEM and resid 1 and name CHB)	3.57	0.14	0.15
35	assign (segid 3A4 and resid 383 and name O)	(segid HEM and resid 1 and name CHC)	7.61	0.19	0.19
	assign (segid 3A4 and resid 383 and name O)	(segid HEM and resid 1 and name CMA)	3.53	0.09	0.09
	assign (segid 3A4 and resid 383 and name O)	(segid HEM and resid 1 and name CMB)	3.53	0.16	0.16
	assign (segid 3A4 and resid 383 and name O)	(segid HEM and resid 1 and name FE)	6.77	0.20	0.19
	assign (segid 3A4 and resid 383 and name O)	(segid HEM and resid 1 and name NA)	5.58	0.14	0.14
40	assign (segid 3A4 and resid 383 and name O)	(segid HEM and resid 1 and name NB)	5.62	0.17	0.18
	assign (segid 3A4 and resid 384 and name C)	(segid 3A4 and resid 384 and name CB)	2.49	0.03	0.04
	assign (segid 3A4 and resid 384 and name C)	(segid 3A4 and resid 384 and name CD1)	4.58	0.15	0.15
	assign (segid 3A4 and resid 384 and name C)	(segid 3A4 and resid 384 and name CD2)	4.75	0.13	0.13
	assign (segid 3A4 and resid 384 and name C)	(segid 3A4 and resid 384 and name CG)	3.85	0.02	0.02
45	assign (segid 3A4 and resid 384 and name C)	(segid 3A4 and resid 384 and name O)	1.22	0.00	0.01
	assign (segid 3A4 and resid 384 and name C)	(segid 3A4 and resid 385 and name C)	3.21	0.07	0.06
	assign (segid 3A4 and resid 384 and name C)	(segid 3A4 and resid 385 and name CA)	2.43	0.02	0.02
	assign (segid 3A4 and resid 384 and name C)	(segid 3A4 and resid 385 and name N)	1.33	0.01	0.00
50	assign (segid 3A4 and resid 384 and name C)	(segid 3A4 and resid 385 and name O)	3.36	0.14	0.14
	assign (segid 3A4 and resid 384 and name C)	(segid 3A4 and resid 386 and name C)	6.46	0.09	0.10
	assign (segid 3A4 and resid 384 and name C)	(segid 3A4 and resid 386 and name CA)	5.44	0.11	0.11
	assign (segid 3A4 and resid 384 and name C)	(segid 3A4 and resid 386 and name N)	4.30	0.06	0.06
	assign (segid 3A4 and resid 384 and name C)	(segid 3A4 and resid 386 and name O)	6.85	0.22	0.22
	assign (segid 3A4 and resid 384 and name C)	(segid 3A4 and resid 387 and name N)	7.17	0.29	0.29
55	assign (segid 3A4 and resid 384 and name C)	(segid 3A4 and resid 389 and name C)	6.41	0.17	0.16
	assign (segid 3A4 and resid 384 and name C)	(segid 3A4 and resid 389 and name O)	5.94	0.19	0.19
	assign (segid 3A4 and resid 384 and name C)	(segid 3A4 and resid 390 and name C)	4.94	0.13	0.12
	assign (segid 3A4 and resid 384 and name C)	(segid 3A4 and resid 390 and name CA)	4.76	0.17	0.17
60	assign (segid 3A4 and resid 384 and name C)	(segid 3A4 and resid 390 and name CB)	5.13	0.30	0.30
	assign (segid 3A4 and resid 384 and name C)	(segid 3A4 and resid 390 and name N)	5.97	0.13	0.14
	assign (segid 3A4 and resid 384 and name C)	(segid 3A4 and resid 390 and name O)	6.12	0.11	0.11
	assign (segid 3A4 and resid 384 and name C)	(segid 3A4 and resid 391 and name C)	6.03	0.07	0.08
	assign (segid 3A4 and resid 384 and name C)	(segid 3A4 and resid 391 and name CA)	4.81	0.09	0.10
	assign (segid 3A4 and resid 384 and name C)	(segid 3A4 and resid 391 and name CB)	4.24	0.13	0.13
65	assign (segid 3A4 and resid 384 and name C)	(segid 3A4 and resid 391 and name N)	4.08	0.09	0.10
	assign (segid 3A4 and resid 384 and name C)	(segid 3A4 and resid 391 and name O)	6.16	0.10	0.10
	assign (segid 3A4 and resid 384 and name C)	(segid 3A4 and resid 392 and name N)	7.18	0.07	0.06
	assign (segid 3A4 and resid 384 and name C)	(segid 3A4 and resid 392 and name CA)	7.39	0.18	0.17
	assign (segid 3A4 and resid 384 and name C)	(segid 3A4 and resid 394 and name CA)	6.56	0.21	0.21
70	assign (segid 3A4 and resid 384 and name C)	(segid 3A4 and resid 394 and name CB)	7.67	0.10	0.10
	assign (segid 3A4 and resid 384 and name C)	(segid 3A4 and resid 394 and name N)	5.15	0.25	0.24
	assign (segid 3A4 and resid 384 and name C)	(segid HEM and resid 1 and name C1A)	5.55	0.15	0.15
	assign (segid 3A4 and resid 384 and name C)	(segid HEM and resid 1 and name C2A)	4.51	0.26	0.27
	assign (segid 3A4 and resid 384 and name C)	(segid HEM and resid 1 and name C2B)	6.23	0.14	0.14
75	assign (segid 3A4 and resid 384 and name C)	(segid HEM and resid 1 and name C3A)	4.00	0.17	0.18
	assign (segid 3A4 and resid 384 and name C)	(segid HEM and resid 1 and name C3B)	7.23	0.16	0.15
	assign (segid 3A4 and resid 384 and name C)	(segid HEM and resid 1 and name C4A)	4.39	0.14	0.14
	assign (segid 3A4 and resid 384 and name C)	(segid HEM and resid 1 and name C4B)	7.24	0.15	0.14
	assign (segid 3A4 and resid 384 and name C)	(segid HEM and resid 1 and name C4D)	7.11	0.21	0.22
80	assign (segid 3A4 and resid 384 and name C)	(segid HEM and resid 1 and name CAA)	4.98	0.32	0.32
	assign (segid 3A4 and resid 384 and name C)	(segid HEM and resid 1 and name CBA)	5.41	0.65	0.65
	assign (segid 3A4 and resid 384 and name C)	(segid HEM and resid 1 and name CGA)	6.19	0.66	0.66

	assign (segid 3A4 and resid 384 and name C) (segid HEM and resid 1 and name CHA)	6.17	0.28	0.28
	assign (segid 3A4 and resid 384 and name C) (segid HEM and resid 1 and name CHB)	4.63	0.10	0.11
	assign (segid 3A4 and resid 384 and name C) (segid HEM and resid 1 and name CMA)	3.88	0.09	0.10
	assign (segid 3A4 and resid 384 and name C) (segid HEM and resid 1 and name CMB)	6.22	0.14	0.14
5	assign (segid 3A4 and resid 384 and name C) (segid HEM and resid 1 and name FE)	6.45	0.24	0.24
	assign (segid 3A4 and resid 384 and name C) (segid HEM and resid 1 and name NA)	5.09	0.17	0.18
	assign (segid 3A4 and resid 384 and name C) (segid HEM and resid 1 and name NB)	6.28	0.14	0.14
	assign (segid 3A4 and resid 384 and name C) (segid HEM and resid 1 and name ND)	7.34	0.20	0.20
	assign (segid 3A4 and resid 384 and name C) (segid HEM and resid 1 and name O1A)	6.32	0.59	0.59
10	assign (segid 3A4 and resid 384 and name CA) (segid 3A4 and resid 384 and name C)	1.53	0.02	0.02
	assign (segid 3A4 and resid 384 and name CA) (segid 3A4 and resid 384 and name CB)	1.52	0.02	0.02
	assign (segid 3A4 and resid 384 and name CA) (segid 3A4 and resid 384 and name CD1)	3.27	0.13	0.12
	assign (segid 3A4 and resid 384 and name CA) (segid 3A4 and resid 384 and name CD2)	3.46	0.10	0.10
	assign (segid 3A4 and resid 384 and name CA) (segid 3A4 and resid 384 and name CG)	2.54	0.03	0.03
15	assign (segid 3A4 and resid 384 and name CA) (segid 3A4 and resid 384 and name O)	2.39	0.03	0.02
	assign (segid 3A4 and resid 384 and name CA) (segid 3A4 and resid 385 and name C)	4.53	0.06	0.07
	assign (segid 3A4 and resid 384 and name CA) (segid 3A4 and resid 385 and name CA)	3.81	0.02	0.02
	assign (segid 3A4 and resid 384 and name CA) (segid 3A4 and resid 385 and name N)	2.44	0.02	0.01
	assign (segid 3A4 and resid 384 and name CA) (segid 3A4 and resid 385 and name O)	4.40	0.14	0.15
20	assign (segid 3A4 and resid 384 and name CA) (segid 3A4 and resid 386 and name CA)	6.77	0.12	0.12
	assign (segid 3A4 and resid 384 and name CA) (segid 3A4 and resid 386 and name N)	5.71	0.06	0.07
	assign (segid 3A4 and resid 384 and name CA) (segid 3A4 and resid 387 and name CA)	9.76	0.23	0.24
	assign (segid 3A4 and resid 384 and name CA) (segid 3A4 and resid 388 and name CA)	11.29	0.13	0.14
	assign (segid 3A4 and resid 384 and name CA) (segid 3A4 and resid 388 and name CB)	12.71	0.09	0.08
25	assign (segid 3A4 and resid 384 and name CA) (segid 3A4 and resid 389 and name C)	7.70	0.13	0.13
	assign (segid 3A4 and resid 384 and name CA) (segid 3A4 and resid 389 and name CA)	9.18	0.15	0.14
	assign (segid 3A4 and resid 384 and name CA) (segid 3A4 and resid 389 and name CB)	9.56	0.24	0.23
	assign (segid 3A4 and resid 384 and name CA) (segid 3A4 and resid 389 and name O)	7.16	0.15	0.15
	assign (segid 3A4 and resid 384 and name CA) (segid 3A4 and resid 390 and name C)	5.86	0.11	0.11
30	assign (segid 3A4 and resid 384 and name CA) (segid 3A4 and resid 390 and name CA)	5.95	0.16	0.15
	assign (segid 3A4 and resid 384 and name CA) (segid 3A4 and resid 390 and name CB)	6.21	0.30	0.30
	assign (segid 3A4 and resid 384 and name CA) (segid 3A4 and resid 390 and name N)	7.25	0.12	0.12
	assign (segid 3A4 and resid 384 and name CA) (segid 3A4 and resid 390 and name O)	6.97	0.09	0.08
	assign (segid 3A4 and resid 384 and name CA) (segid 3A4 and resid 391 and name C)	6.27	0.06	0.06
35	assign (segid 3A4 and resid 384 and name CA) (segid 3A4 and resid 391 and name CA)	5.17	0.04	0.05
	assign (segid 3A4 and resid 384 and name CA) (segid 3A4 and resid 391 and name CB)	4.19	0.08	0.07
	assign (segid 3A4 and resid 384 and name CA) (segid 3A4 and resid 391 and name N)	4.80	0.07	0.07
	assign (segid 3A4 and resid 384 and name CA) (segid 3A4 and resid 391 and name O)	6.30	0.15	0.14
	assign (segid 3A4 and resid 384 and name CA) (segid 3A4 and resid 392 and name CA)	8.63	0.05	0.05
40	assign (segid 3A4 and resid 384 and name CA) (segid 3A4 and resid 392 and name CB)	9.87	0.06	0.05
	assign (segid 3A4 and resid 384 and name CA) (segid 3A4 and resid 392 and name N)	7.43	0.04	0.04
	assign (segid 3A4 and resid 384 and name CA) (segid 3A4 and resid 393 and name CA)	8.76	0.08	0.07
	assign (segid 3A4 and resid 384 and name CA) (segid 3A4 and resid 394 and name CA)	6.59	0.17	0.17
	assign (segid 3A4 and resid 384 and name CA) (segid 3A4 and resid 394 and name CB)	5.89	0.21	0.22
45	assign (segid 3A4 and resid 384 and name CA) (segid 3A4 and resid 394 and name N)	7.07	0.11	0.10
	assign (segid 3A4 and resid 384 and name CA) (segid 3A4 and resid 395 and name CA)	10.15	0.25	0.25
	assign (segid 3A4 and resid 384 and name CA) (segid 3A4 and resid 396 and name CA)	11.80	0.14	0.14
	assign (segid 3A4 and resid 384 and name CA) (segid 3A4 and resid 396 and name CB)	12.17	0.23	0.23
	assign (segid 3A4 and resid 384 and name CA) (segid 3A4 and resid 397 and name CA)	9.73	0.20	0.20
50	assign (segid 3A4 and resid 384 and name CA) (segid 3A4 and resid 397 and name CB)	8.33	0.23	0.22
	assign (segid 3A4 and resid 384 and name CA) (segid 3A4 and resid 398 and name CA)	10.43	0.28	0.28
	assign (segid 3A4 and resid 384 and name CA) (segid 3A4 and resid 398 and name CB)	10.07	0.26	0.27
	assign (segid 3A4 and resid 384 and name CA) (segid 3A4 and resid 399 and name CA)	13.94	0.24	0.23
	assign (segid 3A4 and resid 384 and name CA) (segid 3A4 and resid 399 and name CB)	14.45	0.20	0.20
55	assign (segid 3A4 and resid 384 and name CA) (segid 3A4 and resid 400 and name CA)	14.71	0.26	0.26
	assign (segid 3A4 and resid 384 and name CA) (segid 3A4 and resid 400 and name CB)	14.21	0.30	0.29
	assign (segid 3A4 and resid 384 and name CA) (segid 3A4 and resid 401 and name CA)	13.81	0.28	0.27
	assign (segid 3A4 and resid 384 and name CA) (segid 3A4 and resid 402 and name CA)	15.83	0.22	0.22
	assign (segid 3A4 and resid 384 and name CA) (segid 3A4 and resid 402 and name CB)	15.61	0.21	0.21
60	assign (segid 3A4 and resid 384 and name CA) (segid 3A4 and resid 403 and name CA)	18.61	0.26	0.26
	assign (segid 3A4 and resid 384 and name CA) (segid 3A4 and resid 403 and name CB)	18.67	0.24	0.24
	assign (segid 3A4 and resid 384 and name CA) (segid 3A4 and resid 404 and name CA)	18.98	0.28	0.28
	assign (segid 3A4 and resid 384 and name CA) (segid 3A4 and resid 404 and name CB)	18.08	0.30	0.31
	assign (segid 3A4 and resid 384 and name CA) (segid 3A4 and resid 405 and name CA)	19.12	0.28	0.27
65	assign (segid 3A4 and resid 384 and name CA) (segid 3A4 and resid 405 and name CB)	18.07	0.31	0.31
	assign (segid 3A4 and resid 384 and name CA) (segid 3A4 and resid 431 and name CA)	14.33	1.22	1.21
	assign (segid 3A4 and resid 384 and name CA) (segid 3A4 and resid 433 and name CA)	14.21	0.16	0.16
	assign (segid 3A4 and resid 384 and name CA) (segid 3A4 and resid 434 and name CA)	15.81	0.65	0.64
	assign (segid 3A4 and resid 384 and name CA) (segid 3A4 and resid 435 and name CA)	18.78	0.61	0.61
70	assign (segid 3A4 and resid 384 and name CA) (segid HEM and resid 1 and name C1A)	5.57	0.17	0.16
	assign (segid 3A4 and resid 384 and name CA) (segid HEM and resid 1 and name C1B)	4.76	0.09	0.09
	assign (segid 3A4 and resid 384 and name CA) (segid HEM and resid 1 and name C2A)	5.14	0.19	0.18
	assign (segid 3A4 and resid 384 and name CA) (segid HEM and resid 1 and name C2B)	5.15	0.10	0.11
	assign (segid 3A4 and resid 384 and name CA) (segid HEM and resid 1 and name C3A)	4.34	0.12	0.13
75	assign (segid 3A4 and resid 384 and name CA) (segid HEM and resid 1 and name C3B)	6.12	0.13	0.13
	assign (segid 3A4 and resid 384 and name CA) (segid HEM and resid 1 and name C4A)	4.30	0.09	0.10
	assign (segid 3A4 and resid 384 and name CA) (segid HEM and resid 1 and name C4B)	6.34	0.12	0.11
	assign (segid 3A4 and resid 384 and name CA) (segid HEM and resid 1 and name C4D)	7.48	0.14	0.14
	assign (segid 3A4 and resid 384 and name CA) (segid HEM and resid 1 and name CAA)	5.94	0.25	0.24
80	assign (segid 3A4 and resid 384 and name CA) (segid HEM and resid 1 and name CAB)	7.11	0.12	0.13
	assign (segid 3A4 and resid 384 and name CA) (segid HEM and resid 1 and name CBA)	6.47	0.61	0.60
	assign (segid 3A4 and resid 384 and name CA) (segid HEM and resid 1 and name CHA)	6.70	0.18	0.18
	assign (segid 3A4 and resid 384 and name CA) (segid HEM and resid 1 and name CHB)	4.10	0.06	0.06

	assign (segid 3A4 and resid 384 and name CA)	(segid HEM and resid 1 and name CHC)	7.46	0.13	0.12
	assign (segid 3A4 and resid 384 and name CA)	(segid HEM and resid 1 and name CMA)	4.24	0.08	0.08
	assign (segid 3A4 and resid 384 and name CA)	(segid HEM and resid 1 and name CMB)	5.04	0.12	0.12
	assign (segid 3A4 and resid 384 and name CA)	(segid HEM and resid 1 and name FE)	6.17	0.16	0.17
5	assign (segid 3A4 and resid 384 and name CA)	(segid HEM and resid 1 and name NA)	5.12	0.11	0.11
	assign (segid 3A4 and resid 384 and name CA)	(segid HEM and resid 1 and name NB)	5.59	0.09	0.09
	assign (segid 3A4 and resid 384 and name CA)	(segid HEM and resid 1 and name NC)	7.72	0.12	0.11
	assign (segid 3A4 and resid 384 and name CA)	(segid HEM and resid 1 and name ND)	7.42	0.14	0.14
	assign (segid 3A4 and resid 384 and name CB)	(segid 3A4 and resid 384 and name CD1)	2.52	0.01	0.01
10	assign (segid 3A4 and resid 384 and name CB)	(segid 3A4 and resid 384 and name CD2)	2.51	0.02	0.01
	assign (segid 3A4 and resid 384 and name CB)	(segid 3A4 and resid 384 and name CG)	1.51	0.01	0.01
	assign (segid 3A4 and resid 384 and name CB)	(segid 3A4 and resid 385 and name C)	5.20	0.11	0.10
	assign (segid 3A4 and resid 384 and name CB)	(segid 3A4 and resid 385 and name CA)	4.82	0.04	0.04
	assign (segid 3A4 and resid 384 and name CB)	(segid 3A4 and resid 385 and name N)	3.59	0.01	0.01
15	assign (segid 3A4 and resid 384 and name CB)	(segid 3A4 and resid 385 and name O)	4.85	0.20	0.21
	assign (segid 3A4 and resid 384 and name CB)	(segid 3A4 and resid 386 and name CA)	7.13	0.18	0.19
	assign (segid 3A4 and resid 384 and name CB)	(segid 3A4 and resid 386 and name N)	6.29	0.10	0.11
	assign (segid 3A4 and resid 384 and name CB)	(segid 3A4 and resid 387 and name CA)	9.91	0.29	0.28
	assign (segid 3A4 and resid 384 and name CB)	(segid 3A4 and resid 388 and name CA)	11.27	0.22	0.21
20	assign (segid 3A4 and resid 384 and name CB)	(segid 3A4 and resid 388 and name CB)	12.72	0.18	0.19
	assign (segid 3A4 and resid 384 and name CB)	(segid 3A4 and resid 389 and name CA)	9.41	0.12	0.13
	assign (segid 3A4 and resid 384 and name CB)	(segid 3A4 and resid 389 and name CB)	10.01	0.21	0.20
	assign (segid 3A4 and resid 384 and name CB)	(segid 3A4 and resid 389 and name O)	7.46	0.16	0.17
	assign (segid 3A4 and resid 384 and name CB)	(segid 3A4 and resid 390 and name C)	5.63	0.13	0.14
25	assign (segid 3A4 and resid 384 and name CB)	(segid 3A4 and resid 390 and name CA)	5.88	0.17	0.16
	assign (segid 3A4 and resid 384 and name CB)	(segid 3A4 and resid 390 and name CB)	5.88	0.30	0.31
	assign (segid 3A4 and resid 384 and name CB)	(segid 3A4 and resid 390 and name N)	7.28	0.15	0.15
	assign (segid 3A4 and resid 384 and name CB)	(segid 3A4 and resid 390 and name O)	6.64	0.13	0.14
	assign (segid 3A4 and resid 384 and name CB)	(segid 3A4 and resid 391 and name C)	5.61	0.12	0.12
30	assign (segid 3A4 and resid 384 and name CB)	(segid 3A4 and resid 391 and name CA)	4.82	0.08	0.07
	assign (segid 3A4 and resid 384 and name CB)	(segid 3A4 and resid 391 and name CB)	3.78	0.07	0.08
	assign (segid 3A4 and resid 384 and name CB)	(segid 3A4 and resid 391 and name N)	4.55	0.11	0.11
	assign (segid 3A4 and resid 384 and name CB)	(segid 3A4 and resid 391 and name O)	5.39	0.22	0.22
	assign (segid 3A4 and resid 384 and name CB)	(segid 3A4 and resid 392 and name CA)	7.88	0.11	0.11
35	assign (segid 3A4 and resid 384 and name CB)	(segid 3A4 and resid 392 and name CB)	9.24	0.10	0.10
	assign (segid 3A4 and resid 384 and name CB)	(segid 3A4 and resid 392 and name N)	6.83	0.08	0.09
	assign (segid 3A4 and resid 384 and name CB)	(segid 3A4 and resid 393 and name C)	7.02	0.20	0.21
	assign (segid 3A4 and resid 384 and name CB)	(segid 3A4 and resid 393 and name CA)	7.89	0.17	0.16
	assign (segid 3A4 and resid 384 and name CB)	(segid 3A4 and resid 393 and name N)	7.50	0.15	0.16
40	assign (segid 3A4 and resid 384 and name CB)	(segid 3A4 and resid 394 and name C)	6.52	0.30	0.29
	assign (segid 3A4 and resid 384 and name CB)	(segid 3A4 and resid 394 and name CA)	5.33	0.26	0.25
	assign (segid 3A4 and resid 384 and name CB)	(segid 3A4 and resid 394 and name CB)	4.49	0.27	0.28
	assign (segid 3A4 and resid 384 and name CB)	(segid 3A4 and resid 394 and name N)	5.95	0.21	0.21
	assign (segid 3A4 and resid 384 and name CB)	(segid 3A4 and resid 394 and name O)	6.75	0.30	0.30
45	assign (segid 3A4 and resid 384 and name CB)	(segid 3A4 and resid 395 and name CA)	8.76	0.32	0.33
	assign (segid 3A4 and resid 384 and name CB)	(segid 3A4 and resid 396 and name CA)	10.67	0.25	0.25
	assign (segid 3A4 and resid 384 and name CB)	(segid 3A4 and resid 396 and name CB)	11.13	0.30	0.30
	assign (segid 3A4 and resid 384 and name CB)	(segid 3A4 and resid 397 and name CA)	8.85	0.27	0.27
	assign (segid 3A4 and resid 384 and name CB)	(segid 3A4 and resid 397 and name CB)	7.54	0.28	0.28
50	assign (segid 3A4 and resid 384 and name CB)	(segid 3A4 and resid 398 and name CA)	9.35	0.32	0.31
	assign (segid 3A4 and resid 384 and name CB)	(segid 3A4 and resid 398 and name CB)	8.88	0.31	0.30
	assign (segid 3A4 and resid 384 and name CB)	(segid 3A4 and resid 398 and name CG)	7.57	0.26	0.27
	assign (segid 3A4 and resid 384 and name CB)	(segid 3A4 and resid 399 and name CA)	12.78	0.29	0.28
	assign (segid 3A4 and resid 384 and name CB)	(segid 3A4 and resid 399 and name CB)	13.25	0.27	0.26
55	assign (segid 3A4 and resid 384 and name CB)	(segid 3A4 and resid 400 and name CA)	13.83	0.28	0.29
	assign (segid 3A4 and resid 384 and name CB)	(segid 3A4 and resid 400 and name CB)	13.42	0.31	0.31
	assign (segid 3A4 and resid 384 and name CB)	(segid 3A4 and resid 401 and name CA)	13.11	0.29	0.28
	assign (segid 3A4 and resid 384 and name CB)	(segid 3A4 and resid 402 and name CA)	14.92	0.25	0.24
	assign (segid 3A4 and resid 384 and name CB)	(segid 3A4 and resid 402 and name CB)	14.59	0.24	0.24
60	assign (segid 3A4 and resid 384 and name CB)	(segid 3A4 and resid 403 and name CA)	17.68	0.30	0.29
	assign (segid 3A4 and resid 384 and name CB)	(segid 3A4 and resid 403 and name CB)	17.70	0.29	0.29
	assign (segid 3A4 and resid 384 and name CB)	(segid 3A4 and resid 404 and name CA)	18.30	0.30	0.30
	assign (segid 3A4 and resid 384 and name CB)	(segid 3A4 and resid 404 and name CB)	17.48	0.31	0.32
	assign (segid 3A4 and resid 384 and name CB)	(segid 3A4 and resid 405 and name CA)	18.51	0.27	0.27
65	assign (segid 3A4 and resid 384 and name CB)	(segid 3A4 and resid 405 and name CB)	17.49	0.30	0.29
	assign (segid 3A4 and resid 384 and name CB)	(segid 3A4 and resid 431 and name CA)	15.62	1.18	1.17
	assign (segid 3A4 and resid 384 and name CB)	(segid 3A4 and resid 433 and name CA)	15.28	0.16	0.16
	assign (segid 3A4 and resid 384 and name CB)	(segid 3A4 and resid 434 and name CA)	16.65	0.62	0.62
	assign (segid 3A4 and resid 384 and name CB)	(segid HEM and resid 1 and name C1A)	6.16	0.20	0.21
70	assign (segid 3A4 and resid 384 and name CB)	(segid HEM and resid 1 and name C1B)	5.20	0.13	0.12
	assign (segid 3A4 and resid 384 and name CB)	(segid HEM and resid 1 and name C2A)	6.03	0.20	0.20
	assign (segid 3A4 and resid 384 and name CB)	(segid HEM and resid 1 and name C2B)	5.50	0.11	0.12
	assign (segid 3A4 and resid 384 and name CB)	(segid HEM and resid 1 and name C3A)	5.40	0.14	0.14
	assign (segid 3A4 and resid 384 and name CB)	(segid HEM and resid 1 and name C3B)	6.19	0.13	0.13
75	assign (segid 3A4 and resid 384 and name CB)	(segid HEM and resid 1 and name C4A)	5.10	0.15	0.15
	assign (segid 3A4 and resid 384 and name CB)	(segid HEM and resid 1 and name C4B)	6.32	0.14	0.15
	assign (segid 3A4 and resid 384 and name CB)	(segid HEM and resid 1 and name CAA)	6.89	0.25	0.26
	assign (segid 3A4 and resid 384 and name CB)	(segid HEM and resid 1 and name CAB)	7.05	0.11	0.10
	assign (segid 3A4 and resid 384 and name CB)	(segid HEM and resid 1 and name CHA)	7.13	0.23	0.22
80	assign (segid 3A4 and resid 384 and name CB)	(segid HEM and resid 1 and name CHB)	4.87	0.14	0.14
	assign (segid 3A4 and resid 384 and name CB)	(segid HEM and resid 1 and name CHC)	7.25	0.16	0.17
	assign (segid 3A4 and resid 384 and name CB)	(segid HEM and resid 1 and name CMA)	5.59	0.11	0.11
	assign (segid 3A4 and resid 384 and name CB)	(segid HEM and resid 1 and name CMB)	5.59	0.13	0.13

	assign (segid 3A4 and resid 384 and name CB)	(segid HEM and resid 1 and name FE)	6.27	0.19	0.19
	assign (segid 3A4 and resid 384 and name CB)	(segid HEM and resid 1 and name NA)	5.63	0.16	0.16
	assign (segid 3A4 and resid 384 and name CB)	(segid HEM and resid 1 and name NB)	5.77	0.13	0.13
	assign (segid 3A4 and resid 384 and name CB)	(segid HEM and resid 1 and name NC)	7.57	0.16	0.15
	assign (segid 3A4 and resid 384 and name CB)	(segid HEM and resid 1 and name ND)	7.51	0.17	0.17
5	assign (segid 3A4 and resid 384 and name CB)	(segid HEM and resid 1 and name ND)	2.40	0.01	0.02
	assign (segid 3A4 and resid 384 and name CD1)	(segid 3A4 and resid 384 and name CD2)	7.37	0.18	0.18
	assign (segid 3A4 and resid 384 and name CD1)	(segid 3A4 and resid 385 and name C)	6.88	0.08	0.07
	assign (segid 3A4 and resid 384 and name CD1)	(segid 3A4 and resid 385 and name CA)	5.55	0.05	0.06
	assign (segid 3A4 and resid 384 and name CD1)	(segid 3A4 and resid 385 and name N)	6.97	0.42	0.42
10	assign (segid 3A4 and resid 384 and name CD1)	(segid 3A4 and resid 391 and name C)	6.59	0.64	0.64
	assign (segid 3A4 and resid 384 and name CD1)	(segid 3A4 and resid 391 and name CA)	6.02	0.66	0.66
	assign (segid 3A4 and resid 384 and name CD1)	(segid 3A4 and resid 391 and name CB)	4.66	0.76	0.75
	assign (segid 3A4 and resid 384 and name CD1)	(segid 3A4 and resid 391 and name N)	6.24	0.53	0.53
	assign (segid 3A4 and resid 384 and name CD1)	(segid 3A4 and resid 391 and name O)	6.34	0.64	0.64
15	assign (segid 3A4 and resid 384 and name CD1)	(segid 3A4 and resid 393 and name C)	6.35	0.59	0.58
	assign (segid 3A4 and resid 384 and name CD1)	(segid 3A4 and resid 393 and name O)	6.56	0.56	0.56
	assign (segid 3A4 and resid 384 and name CD1)	(segid 3A4 and resid 393 and name C)	5.51	0.14	0.15
	assign (segid 3A4 and resid 384 and name CD1)	(segid 3A4 and resid 394 and name CA)	4.61	0.29	0.30
	assign (segid 3A4 and resid 384 and name CD1)	(segid 3A4 and resid 394 and name CB)	4.28	0.24	0.24
20	assign (segid 3A4 and resid 384 and name CD1)	(segid 3A4 and resid 394 and name N)	5.50	0.48	0.48
	assign (segid 3A4 and resid 384 and name CD1)	(segid 3A4 and resid 394 and name O)	5.40	0.15	0.14
	assign (segid 3A4 and resid 384 and name CD1)	(segid 3A4 and resid 394 and name N)	6.70	0.15	0.15
	assign (segid 3A4 and resid 384 and name CD1)	(segid 3A4 and resid 397 and name C)	7.23	0.15	0.15
	assign (segid 3A4 and resid 384 and name CD1)	(segid 3A4 and resid 397 and name CA)	7.07	0.30	0.29
25	assign (segid 3A4 and resid 384 and name CD1)	(segid 3A4 and resid 397 and name CB)	5.79	0.38	0.38
	assign (segid 3A4 and resid 384 and name CD1)	(segid 3A4 and resid 398 and name CA)	7.42	0.35	0.36
	assign (segid 3A4 and resid 384 and name CD1)	(segid 3A4 and resid 398 and name CB)	7.11	0.44	0.45
	assign (segid 3A4 and resid 384 and name CD1)	(segid 3A4 and resid 398 and name CD1)	6.02	0.67	0.67
	assign (segid 3A4 and resid 384 and name CD1)	(segid 3A4 and resid 398 and name CG)	5.83	0.52	0.51
30	assign (segid 3A4 and resid 384 and name CD1)	(segid 3A4 and resid 398 and name N)	6.88	0.20	0.21
	assign (segid 3A4 and resid 384 and name CD1)	(segid 3A4 and resid 398 and name N)	4.75	0.78	0.78
	assign (segid 3A4 and resid 384 and name CD1)	(segid HEM and resid 1 and name C1B)	4.54	0.68	0.68
	assign (segid 3A4 and resid 384 and name CD1)	(segid HEM and resid 1 and name C2B)	6.45	0.60	0.59
	assign (segid 3A4 and resid 384 and name CD1)	(segid HEM and resid 1 and name C3A)	4.92	0.72	0.73
35	assign (segid 3A4 and resid 384 and name CD1)	(segid HEM and resid 1 and name C3B)	5.70	0.70	0.70
	assign (segid 3A4 and resid 384 and name CD1)	(segid HEM and resid 1 and name C4A)	5.34	0.81	0.81
	assign (segid 3A4 and resid 384 and name CD1)	(segid HEM and resid 1 and name C4B)	5.45	0.67	0.67
	assign (segid 3A4 and resid 384 and name CD1)	(segid HEM and resid 1 and name CBB)	5.69	0.46	0.46
	assign (segid 3A4 and resid 384 and name CD1)	(segid HEM and resid 1 and name CHB)	5.00	0.70	0.69
40	assign (segid 3A4 and resid 384 and name CD1)	(segid HEM and resid 1 and name CHC)	6.19	0.83	0.82
	assign (segid 3A4 and resid 384 and name CD1)	(segid HEM and resid 1 and name CMA)	6.69	0.44	0.45
	assign (segid 3A4 and resid 384 and name CD1)	(segid HEM and resid 1 and name CMB)	4.63	0.42	0.42
	assign (segid 3A4 and resid 384 and name CD1)	(segid HEM and resid 1 and name FE)	6.30	0.97	0.97
	assign (segid 3A4 and resid 384 and name CD1)	(segid HEM and resid 1 and name NA)	6.22	0.81	0.80
45	assign (segid 3A4 and resid 384 and name CD1)	(segid HEM and resid 1 and name NB)	5.26	0.84	0.83
	assign (segid 3A4 and resid 384 and name CD1)	(segid HEM and resid 1 and name NB)	7.52	0.08	0.07
	assign (segid 3A4 and resid 384 and name CD2)	(segid 3A4 and resid 385 and name CA)	7.09	0.05	0.06
	assign (segid 3A4 and resid 384 and name CD2)	(segid 3A4 and resid 385 and name N)	5.77	0.05	0.05
50	assign (segid 3A4 and resid 384 and name CD2)	(segid 3A4 and resid 385 and name O)	7.08	0.14	0.14
	assign (segid 3A4 and resid 384 and name CD2)	(segid 3A4 and resid 390 and name C)	7.30	0.39	0.39
	assign (segid 3A4 and resid 384 and name CD2)	(segid 3A4 and resid 391 and name C)	6.36	0.56	0.56
	assign (segid 3A4 and resid 384 and name CD2)	(segid 3A4 and resid 391 and name CA)	5.89	0.62	0.61
	assign (segid 3A4 and resid 384 and name CD2)	(segid 3A4 and resid 391 and name CB)	4.56	0.70	0.69
	assign (segid 3A4 and resid 384 and name CD2)	(segid 3A4 and resid 391 and name N)	6.12	0.44	0.44
55	assign (segid 3A4 and resid 384 and name CD2)	(segid 3A4 and resid 391 and name O)	6.06	0.40	0.40
	assign (segid 3A4 and resid 384 and name CD2)	(segid 3A4 and resid 393 and name C)	6.15	0.72	0.73
	assign (segid 3A4 and resid 384 and name CD2)	(segid 3A4 and resid 393 and name O)	6.42	0.71	0.71
	assign (segid 3A4 and resid 384 and name CD2)	(segid 3A4 and resid 393 and name C)	5.28	0.43	0.42
	assign (segid 3A4 and resid 384 and name CD2)	(segid 3A4 and resid 394 and name CA)	4.34	0.53	0.54
60	assign (segid 3A4 and resid 384 and name CD2)	(segid 3A4 and resid 394 and name CB)	3.97	0.34	0.34
	assign (segid 3A4 and resid 384 and name CD2)	(segid 3A4 and resid 394 and name N)	5.25	0.68	0.67
	assign (segid 3A4 and resid 384 and name CD2)	(segid 3A4 and resid 394 and name O)	5.21	0.36	0.35
	assign (segid 3A4 and resid 384 and name CD2)	(segid 3A4 and resid 395 and name N)	6.45	0.41	0.40
65	assign (segid 3A4 and resid 384 and name CD2)	(segid 3A4 and resid 397 and name CB)	5.72	0.75	0.75
	assign (segid 3A4 and resid 384 and name CD2)	(segid 3A4 and resid 398 and name CA)	7.38	0.24	0.23
	assign (segid 3A4 and resid 384 and name CD2)	(segid 3A4 and resid 398 and name CB)	7.03	0.10	0.11
	assign (segid 3A4 and resid 384 and name CD2)	(segid 3A4 and resid 398 and name CD1)	5.91	0.34	0.33
	assign (segid 3A4 and resid 384 and name CD2)	(segid 3A4 and resid 398 and name CG)	5.79	0.18	0.17
	assign (segid 3A4 and resid 384 and name CD2)	(segid 3A4 and resid 398 and name N)	6.81	0.39	0.39
70	assign (segid 3A4 and resid 384 and name CD2)	(segid 3A4 and resid 398 and name N)	4.96	0.93	0.93
	assign (segid 3A4 and resid 384 and name CD2)	(segid HEM and resid 1 and name C1B)	4.81	0.82	0.82
	assign (segid 3A4 and resid 384 and name CD2)	(segid HEM and resid 1 and name C2B)	6.63	0.69	0.68
	assign (segid 3A4 and resid 384 and name CD2)	(segid HEM and resid 1 and name C3A)	5.13	0.86	0.86
	assign (segid 3A4 and resid 384 and name CD2)	(segid HEM and resid 1 and name C3B)	5.88	0.84	0.83
75	assign (segid 3A4 and resid 384 and name CD2)	(segid HEM and resid 1 and name C4A)	5.45	1.01	1.02
	assign (segid 3A4 and resid 384 and name CD2)	(segid HEM and resid 1 and name C4B)	5.64	0.68	0.68
	assign (segid 3A4 and resid 384 and name CD2)	(segid HEM and resid 1 and name CBB)	5.92	0.67	0.68
	assign (segid 3A4 and resid 384 and name CD2)	(segid HEM and resid 1 and name CHB)	5.23	0.85	0.85
	assign (segid 3A4 and resid 384 and name CD2)	(segid HEM and resid 1 and name CHC)	6.23	1.00	0.99
80	assign (segid 3A4 and resid 384 and name CD2)	(segid HEM and resid 1 and name CMA)	6.95	0.54	0.54
	assign (segid 3A4 and resid 384 and name CD2)	(segid HEM and resid 1 and name CMB)	5.00	0.64	0.64
	assign (segid 3A4 and resid 384 and name CD2)	(segid HEM and resid 1 and name FE)	6.33	0.92	0.92

	assign (segid 3A4 and resid 384 and name CD2)	(segid HEM and resid 1 and name NA)	6.31	0.89	0.89
	assign (segid 3A4 and resid 384 and name CD2)	(segid HEM and resid 1 and name NB)	5.38	1.04	1.03
	assign (segid 3A4 and resid 384 and name CG)	(segid 3A4 and resid 384 and name CD1)	1.38	0.01	0.01
	assign (segid 3A4 and resid 384 and name CG)	(segid 3A4 and resid 384 and name CD2)	1.39	0.01	0.02
5	assign (segid 3A4 and resid 384 and name CG)	(segid 3A4 and resid 385 and name C)	6.66	0.10	0.10
	assign (segid 3A4 and resid 384 and name CG)	(segid 3A4 and resid 385 and name CA)	6.22	0.02	0.02
	assign (segid 3A4 and resid 384 and name CG)	(segid 3A4 and resid 385 and name N)	4.90	0.02	0.01
	assign (segid 3A4 and resid 384 and name CG)	(segid 3A4 and resid 385 and name O)	6.27	0.22	0.21
	assign (segid 3A4 and resid 384 and name CG)	(segid 3A4 and resid 386 and name N)	7.79	0.10	0.10
	assign (segid 3A4 and resid 384 and name CG)	(segid 3A4 and resid 390 and name C)	6.72	0.10	0.10
10	assign (segid 3A4 and resid 384 and name CG)	(segid 3A4 and resid 390 and name CA)	7.17	0.13	0.14
	assign (segid 3A4 and resid 384 and name CG)	(segid 3A4 and resid 390 and name CB)	7.17	0.28	0.29
	assign (segid 3A4 and resid 384 and name CG)	(segid 3A4 and resid 390 and name O)	7.61	0.09	0.09
	assign (segid 3A4 and resid 384 and name CG)	(segid 3A4 and resid 391 and name C)	6.07	0.08	0.09
	assign (segid 3A4 and resid 384 and name CG)	(segid 3A4 and resid 391 and name CA)	5.47	0.04	0.04
15	assign (segid 3A4 and resid 384 and name CG)	(segid 3A4 and resid 391 and name CB)	4.18	0.04	0.05
	assign (segid 3A4 and resid 384 and name CG)	(segid 3A4 and resid 391 and name N)	5.55	0.10	0.10
	assign (segid 3A4 and resid 384 and name CG)	(segid 3A4 and resid 391 and name O)	5.80	0.24	0.24
	assign (segid 3A4 and resid 384 and name CG)	(segid 3A4 and resid 392 and name N)	7.21	0.10	0.10
20	assign (segid 3A4 and resid 384 and name CG)	(segid 3A4 and resid 393 and name C)	6.37	0.15	0.16
	assign (segid 3A4 and resid 384 and name CG)	(segid 3A4 and resid 393 and name CA)	7.43	0.13	0.12
	assign (segid 3A4 and resid 384 and name CG)	(segid 3A4 and resid 393 and name N)	7.33	0.14	0.13
	assign (segid 3A4 and resid 384 and name CG)	(segid 3A4 and resid 393 and name O)	6.73	0.21	0.21
	assign (segid 3A4 and resid 384 and name CG)	(segid 3A4 and resid 394 and name C)	5.59	0.24	0.25
25	assign (segid 3A4 and resid 384 and name CG)	(segid 3A4 and resid 394 and name CA)	4.56	0.20	0.20
	assign (segid 3A4 and resid 384 and name CG)	(segid 3A4 and resid 394 and name CB)	4.00	0.23	0.24
	assign (segid 3A4 and resid 384 and name CG)	(segid 3A4 and resid 394 and name N)	5.40	0.16	0.16
	assign (segid 3A4 and resid 384 and name CG)	(segid 3A4 and resid 394 and name O)	5.62	0.27	0.26
	assign (segid 3A4 and resid 384 and name CG)	(segid 3A4 and resid 395 and name N)	6.73	0.24	0.25
30	assign (segid 3A4 and resid 384 and name CG)	(segid 3A4 and resid 397 and name CB)	6.23	0.29	0.29
	assign (segid 3A4 and resid 384 and name CG)	(segid 3A4 and resid 398 and name CB)	7.56	0.26	0.26
	assign (segid 3A4 and resid 384 and name CG)	(segid 3A4 and resid 398 and name CD1)	6.33	0.27	0.28
	assign (segid 3A4 and resid 384 and name CG)	(segid 3A4 and resid 398 and name CG)	6.27	0.22	0.22
	assign (segid 3A4 and resid 384 and name CG)	(segid 3A4 and resid 398 and name N)	7.36	0.29	0.29
35	assign (segid 3A4 and resid 384 and name CG)	(segid HEM and resid 1 and name C1A)	6.76	0.14	0.15
	assign (segid 3A4 and resid 384 and name CG)	(segid HEM and resid 1 and name C1B)	4.83	0.13	0.13
	assign (segid 3A4 and resid 384 and name CG)	(segid HEM and resid 1 and name C1C)	7.17	0.14	0.15
	assign (segid 3A4 and resid 384 and name CG)	(segid HEM and resid 1 and name C2A)	6.82	0.15	0.15
	assign (segid 3A4 and resid 384 and name CG)	(segid HEM and resid 1 and name C2B)	4.80	0.13	0.12
40	assign (segid 3A4 and resid 384 and name CG)	(segid HEM and resid 1 and name C3A)	6.07	0.13	0.12
	assign (segid 3A4 and resid 384 and name CG)	(segid HEM and resid 1 and name C3B)	5.29	0.12	0.11
	assign (segid 3A4 and resid 384 and name CG)	(segid HEM and resid 1 and name C4A)	5.44	0.13	0.14
	assign (segid 3A4 and resid 384 and name CG)	(segid HEM and resid 1 and name C4B)	5.59	0.13	0.13
	assign (segid 3A4 and resid 384 and name CG)	(segid HEM and resid 1 and name CAB)	5.92	0.08	0.09
45	assign (segid 3A4 and resid 384 and name CG)	(segid HEM and resid 1 and name CBB)	6.23	0.30	0.30
	assign (segid 3A4 and resid 384 and name CG)	(segid HEM and resid 1 and name CHB)	4.89	0.17	0.16
	assign (segid 3A4 and resid 384 and name CG)	(segid HEM and resid 1 and name CHC)	6.46	0.15	0.15
	assign (segid 3A4 and resid 384 and name CG)	(segid HEM and resid 1 and name CMA)	6.31	0.13	0.13
	assign (segid 3A4 and resid 384 and name CG)	(segid HEM and resid 1 and name CMB)	4.89	0.15	0.16
50	assign (segid 3A4 and resid 384 and name CG)	(segid HEM and resid 1 and name FE)	6.20	0.12	0.13
	assign (segid 3A4 and resid 384 and name CG)	(segid HEM and resid 1 and name NA)	5.95	0.11	0.12
	assign (segid 3A4 and resid 384 and name CG)	(segid HEM and resid 1 and name NB)	5.35	0.12	0.12
	assign (segid 3A4 and resid 384 and name CG)	(segid HEM and resid 1 and name NC)	7.20	0.12	0.11
	assign (segid 3A4 and resid 384 and name CG)	(segid HEM and resid 1 and name ND)	7.70	0.09	0.09
55	assign (segid 3A4 and resid 384 and name N)	(segid 3A4 and resid 384 and name C)	2.45	0.04	0.04
	assign (segid 3A4 and resid 384 and name N)	(segid 3A4 and resid 384 and name CA)	1.46	0.01	0.01
	assign (segid 3A4 and resid 384 and name N)	(segid 3A4 and resid 384 and name CB)	2.46	0.03	0.02
	assign (segid 3A4 and resid 384 and name N)	(segid 3A4 and resid 384 and name CD1)	3.61	0.20	0.19
	assign (segid 3A4 and resid 384 and name N)	(segid 3A4 and resid 384 and name CD2)	3.90	0.21	0.21
60	assign (segid 3A4 and resid 384 and name N)	(segid 3A4 and resid 384 and name CG)	3.10	0.07	0.06
	assign (segid 3A4 and resid 384 and name N)	(segid 3A4 and resid 384 and name O)	3.58	0.04	0.04
	assign (segid 3A4 and resid 384 and name N)	(segid 3A4 and resid 385 and name C)	4.76	0.09	0.10
	assign (segid 3A4 and resid 384 and name N)	(segid 3A4 and resid 385 and name CA)	4.11	0.06	0.06
	assign (segid 3A4 and resid 384 and name N)	(segid 3A4 and resid 385 and name N)	2.67	0.06	0.06
65	assign (segid 3A4 and resid 384 and name N)	(segid 3A4 and resid 385 and name O)	4.43	0.13	0.14
	assign (segid 3A4 and resid 384 and name N)	(segid 3A4 and resid 386 and name CA)	7.06	0.11	0.11
	assign (segid 3A4 and resid 384 and name N)	(segid 3A4 and resid 386 and name N)	6.07	0.08	0.08
	assign (segid 3A4 and resid 384 and name N)	(segid 3A4 and resid 390 and name C)	7.19	0.10	0.10
	assign (segid 3A4 and resid 384 and name N)	(segid 3A4 and resid 390 and name CA)	7.10	0.14	0.15
70	assign (segid 3A4 and resid 384 and name N)	(segid 3A4 and resid 390 and name CB)	7.25	0.29	0.29
	assign (segid 3A4 and resid 384 and name N)	(segid 3A4 and resid 391 and name C)	7.70	0.07	0.06
	assign (segid 3A4 and resid 384 and name N)	(segid 3A4 and resid 391 and name CA)	6.62	0.04	0.05
	assign (segid 3A4 and resid 384 and name N)	(segid 3A4 and resid 391 and name CB)	5.61	0.07	0.07
	assign (segid 3A4 and resid 384 and name N)	(segid 3A4 and resid 391 and name N)	6.19	0.06	0.07
75	assign (segid 3A4 and resid 384 and name N)	(segid 3A4 and resid 391 and name O)	7.66	0.16	0.17
	assign (segid 3A4 and resid 384 and name N)	(segid 3A4 and resid 394 and name CB)	6.84	0.26	0.26
	assign (segid 3A4 and resid 384 and name N)	(segid HEM and resid 1 and name C1A)	6.74	0.15	0.16
	assign (segid 3A4 and resid 384 and name N)	(segid HEM and resid 1 and name C1B)	5.48	0.08	0.07
	assign (segid 3A4 and resid 384 and name N)	(segid HEM and resid 1 and name C2A)	6.15	0.19	0.18
80	assign (segid 3A4 and resid 384 and name N)	(segid HEM and resid 1 and name C2B)	5.57	0.10	0.10
	assign (segid 3A4 and resid 384 and name N)	(segid HEM and resid 1 and name C3A)	5.19	0.13	0.13
	assign (segid 3A4 and resid 384 and name N)	(segid HEM and resid 1 and name C3B)	6.63	0.12	0.12
	assign (segid 3A4 and resid 384 and name N)	(segid HEM and resid 1 and name C4A)	5.26	0.10	0.09

	assign (segid 3A4 and resid 384 and name N)	(segid HEM and resid 1 and name C4B)	7.12	0.11	0.12
	assign (segid 3A4 and resid 384 and name N)	(segid HEM and resid 1 and name CAA)	6.86	0.26	0.26
	assign (segid 3A4 and resid 384 and name N)	(segid HEM and resid 1 and name CAB)	7.48	0.13	0.12
	assign (segid 3A4 and resid 384 and name N)	(segid HEM and resid 1 and name CHB)	4.82	0.05	0.05
5	assign (segid 3A4 and resid 384 and name N)	(segid HEM and resid 1 and name CMA)	4.69	0.08	0.07
	assign (segid 3A4 and resid 384 and name N)	(segid HEM and resid 1 and name CMB)	5.05	0.11	0.10
	assign (segid 3A4 and resid 384 and name N)	(segid HEM and resid 1 and name FE)	7.36	0.15	0.15
	assign (segid 3A4 and resid 384 and name N)	(segid HEM and resid 1 and name NA)	6.27	0.11	0.11
	assign (segid 3A4 and resid 384 and name N)	(segid HEM and resid 1 and name NB)	6.50	0.09	0.09
10	assign (segid 3A4 and resid 384 and name O)	(segid 3A4 and resid 384 and name CB)	2.83	0.06	0.05
	assign (segid 3A4 and resid 384 and name O)	(segid 3A4 and resid 384 and name CD1)	4.98	0.28	0.27
	assign (segid 3A4 and resid 384 and name O)	(segid 3A4 and resid 384 and name CD2)	5.05	0.22	0.22
	assign (segid 3A4 and resid 384 and name O)	(segid 3A4 and resid 384 and name CG)	4.21	0.02	0.03
	assign (segid 3A4 and resid 384 and name O)	(segid 3A4 and resid 385 and name C)	3.36	0.11	0.11
15	assign (segid 3A4 and resid 384 and name O)	(segid 3A4 and resid 385 and name CA)	2.77	0.04	0.03
	assign (segid 3A4 and resid 384 and name O)	(segid 3A4 and resid 385 and name N)	2.25	0.02	0.01
	assign (segid 3A4 and resid 384 and name O)	(segid 3A4 and resid 385 and name O)	3.68	0.19	0.19
	assign (segid 3A4 and resid 384 and name O)	(segid 3A4 and resid 386 and name C)	6.06	0.18	0.18
	assign (segid 3A4 and resid 384 and name O)	(segid 3A4 and resid 386 and name CA)	5.26	0.17	0.17
20	assign (segid 3A4 and resid 384 and name O)	(segid 3A4 and resid 386 and name N)	4.16	0.11	0.11
	assign (segid 3A4 and resid 384 and name O)	(segid 3A4 and resid 386 and name O)	6.41	0.27	0.27
	assign (segid 3A4 and resid 384 and name O)	(segid 3A4 and resid 387 and name C)	7.66	0.19	0.19
	assign (segid 3A4 and resid 384 and name O)	(segid 3A4 and resid 387 and name N)	6.67	0.36	0.36
	assign (segid 3A4 and resid 384 and name O)	(segid 3A4 and resid 387 and name O)	7.04	0.19	0.20
25	assign (segid 3A4 and resid 384 and name O)	(segid 3A4 and resid 389 and name C)	5.34	0.14	0.14
	assign (segid 3A4 and resid 384 and name O)	(segid 3A4 and resid 389 and name CA)	6.82	0.14	0.15
	assign (segid 3A4 and resid 384 and name O)	(segid 3A4 and resid 389 and name CB)	7.28	0.21	0.21
	assign (segid 3A4 and resid 384 and name O)	(segid 3A4 and resid 389 and name N)	7.41	0.09	0.08
	assign (segid 3A4 and resid 384 and name O)	(segid 3A4 and resid 389 and name O)	4.89	0.17	0.18
30	assign (segid 3A4 and resid 384 and name O)	(segid 3A4 and resid 390 and name C)	3.72	0.13	0.13
	assign (segid 3A4 and resid 384 and name O)	(segid 3A4 and resid 390 and name CA)	3.64	0.18	0.17
	assign (segid 3A4 and resid 384 and name O)	(segid 3A4 and resid 390 and name CB)	4.13	0.34	0.33
	assign (segid 3A4 and resid 384 and name O)	(segid 3A4 and resid 390 and name N)	4.89	0.13	0.12
	assign (segid 3A4 and resid 384 and name O)	(segid 3A4 and resid 390 and name O)	4.91	0.12	0.11
35	assign (segid 3A4 and resid 384 and name O)	(segid 3A4 and resid 391 and name C)	4.99	0.09	0.09
	assign (segid 3A4 and resid 384 and name O)	(segid 3A4 and resid 391 and name CA)	3.78	0.13	0.12
	assign (segid 3A4 and resid 384 and name O)	(segid 3A4 and resid 391 and name CB)	3.49	0.17	0.17
	assign (segid 3A4 and resid 384 and name O)	(segid 3A4 and resid 391 and name N)	2.90	0.10	0.10
	assign (segid 3A4 and resid 384 and name O)	(segid 3A4 and resid 391 and name O)	5.17	0.10	0.11
40	assign (segid 3A4 and resid 384 and name O)	(segid 3A4 and resid 392 and name C)	7.40	0.08	0.09
	assign (segid 3A4 and resid 384 and name O)	(segid 3A4 and resid 392 and name N)	6.12	0.10	0.09
	assign (segid 3A4 and resid 384 and name O)	(segid 3A4 and resid 393 and name N)	7.71	0.14	0.13
	assign (segid 3A4 and resid 384 and name O)	(segid 3A4 and resid 394 and name CA)	7.01	0.15	0.16
	assign (segid 3A4 and resid 384 and name O)	(segid 3A4 and resid 394 and name CB)	6.16	0.18	0.19
45	assign (segid 3A4 and resid 384 and name O)	(segid 3A4 and resid 394 and name N)	7.11	0.08	0.09
	assign (segid 3A4 and resid 384 and name O)	(segid HEM and resid 1 and name C1A)	4.60	0.28	0.28
	assign (segid 3A4 and resid 384 and name O)	(segid HEM and resid 1 and name C1B)	5.73	0.18	0.17
	assign (segid 3A4 and resid 384 and name O)	(segid HEM and resid 1 and name C2A)	4.16	0.28	0.28
	assign (segid 3A4 and resid 384 and name O)	(segid HEM and resid 1 and name C2B)	6.59	0.15	0.16
50	assign (segid 3A4 and resid 384 and name O)	(segid HEM and resid 1 and name C3A)	4.00	0.19	0.19
	assign (segid 3A4 and resid 384 and name O)	(segid HEM and resid 1 and name C3B)	7.45	0.17	0.18
	assign (segid 3A4 and resid 384 and name O)	(segid HEM and resid 1 and name C3D)	7.42	0.24	0.25
	assign (segid 3A4 and resid 384 and name O)	(segid HEM and resid 1 and name C4A)	4.34	0.16	0.17
	assign (segid 3A4 and resid 384 and name O)	(segid HEM and resid 1 and name C4B)	7.23	0.17	0.17
55	assign (segid 3A4 and resid 384 and name O)	(segid HEM and resid 1 and name C4D)	6.31	0.25	0.26
	assign (segid 3A4 and resid 384 and name O)	(segid HEM and resid 1 and name CAA)	4.56	0.31	0.32
	assign (segid 3A4 and resid 384 and name O)	(segid HEM and resid 1 and name CBA)	4.98	0.78	0.78
	assign (segid 3A4 and resid 384 and name O)	(segid HEM and resid 1 and name CBD)	7.53	0.17	0.17
	assign (segid 3A4 and resid 384 and name O)	(segid HEM and resid 1 and name CGA)	5.75	0.77	0.76
60	assign (segid 3A4 and resid 384 and name O)	(segid HEM and resid 1 and name CHA)	5.42	0.32	0.33
	assign (segid 3A4 and resid 384 and name O)	(segid HEM and resid 1 and name CHB)	4.86	0.12	0.12
	assign (segid 3A4 and resid 384 and name O)	(segid HEM and resid 1 and name CMA)	4.27	0.10	0.10
	assign (segid 3A4 and resid 384 and name O)	(segid HEM and resid 1 and name CMB)	6.85	0.15	0.15
	assign (segid 3A4 and resid 384 and name O)	(segid HEM and resid 1 and name FE)	6.01	0.28	0.29
65	assign (segid 3A4 and resid 384 and name O)	(segid HEM and resid 1 and name NA)	4.72	0.21	0.22
	assign (segid 3A4 and resid 384 and name O)	(segid HEM and resid 1 and name NB)	6.21	0.18	0.17
	assign (segid 3A4 and resid 384 and name O)	(segid HEM and resid 1 and name ND)	6.64	0.24	0.23
	assign (segid 3A4 and resid 384 and name O)	(segid HEM and resid 1 and name O1A)	5.89	0.59	0.60
	assign (segid 3A4 and resid 384 and name O)	(segid HEM and resid 1 and name O2A)	6.47	1.18	1.18
70	assign (segid 3A4 and resid 385 and name C)	(segid 3A4 and resid 385 and name O)	1.24	0.01	0.00
	assign (segid 3A4 and resid 385 and name C)	(segid 3A4 and resid 386 and name C)	3.67	0.03	0.04
	assign (segid 3A4 and resid 385 and name C)	(segid 3A4 and resid 386 and name CA)	2.43	0.03	0.03
	assign (segid 3A4 and resid 385 and name C)	(segid 3A4 and resid 386 and name N)	1.34	0.02	0.01
	assign (segid 3A4 and resid 385 and name C)	(segid 3A4 and resid 386 and name O)	4.18	0.22	0.22
75	assign (segid 3A4 and resid 385 and name C)	(segid 3A4 and resid 387 and name C)	6.39	0.06	0.06
	assign (segid 3A4 and resid 385 and name C)	(segid 3A4 and resid 387 and name CA)	5.88	0.14	0.14
	assign (segid 3A4 and resid 385 and name C)	(segid 3A4 and resid 387 and name N)	4.55	0.18	0.19
	assign (segid 3A4 and resid 385 and name C)	(segid 3A4 and resid 387 and name O)	6.14	0.11	0.12
	assign (segid 3A4 and resid 385 and name C)	(segid 3A4 and resid 388 and name N)	7.43	0.06	0.05
80	assign (segid 3A4 and resid 385 and name C)	(segid 3A4 and resid 389 and name C)	5.93	0.27	0.28
	assign (segid 3A4 and resid 385 and name C)	(segid 3A4 and resid 389 and name CA)	7.05	0.28	0.27
	assign (segid 3A4 and resid 385 and name C)	(segid 3A4 and resid 389 and name N)	7.11	0.21	0.22
	assign (segid 3A4 and resid 385 and name C)	(segid 3A4 and resid 389 and name O)	5.96	0.35	0.35

assign (segid 3A4 and resid 385 and name C) (segid 3A4 and resid 390 and name C) 5.62 0.12 0.13
 assign (segid 3A4 and resid 385 and name C) (segid 3A4 and resid 390 and name CA) 4.57 0.19 0.18
 assign (segid 3A4 and resid 385 and name C) (segid 3A4 and resid 390 and name CB) 4.62 0.26 0.26
 assign (segid 3A4 and resid 385 and name C) (segid 3A4 and resid 390 and name N) 5.34 0.21 0.20
 5 assign (segid 3A4 and resid 385 and name C) (segid 3A4 and resid 390 and name O) 6.78 0.14 0.15
 assign (segid 3A4 and resid 385 and name C) (segid 3A4 and resid 391 and name C) 7.84 0.05 0.06
 assign (segid 3A4 and resid 385 and name C) (segid 3A4 and resid 391 and name CA) 6.76 0.05 0.05
 assign (segid 3A4 and resid 385 and name C) (segid 3A4 and resid 391 and name CB) 6.79 0.08 0.08
 assign (segid 3A4 and resid 385 and name C) (segid 3A4 and resid 391 and name N) 5.51 0.07 0.07
 10 assign (segid 3A4 and resid 385 and name C) (segid 3A4 and resid 391 and name O) 7.20 0.29 0.30
 assign (segid 3A4 and resid 385 and name C) (segid HEM and resid 1 and name C1A) 6.27 0.35 0.34
 assign (segid 3A4 and resid 385 and name C) (segid HEM and resid 1 and name C2A) 6.16 0.23 0.24
 assign (segid 3A4 and resid 385 and name C) (segid HEM and resid 1 and name C3A) 7.04 0.15 0.15
 assign (segid 3A4 and resid 385 and name C) (segid HEM and resid 1 and name C4A) 5.91 0.48 0.49
 assign (segid 3A4 and resid 385 and name C) (segid HEM and resid 1 and name CAA) 5.97 0.62 0.62
 15 assign (segid 3A4 and resid 385 and name C) (segid HEM and resid 1 and name CBA) 5.96 0.72 0.72
 assign (segid 3A4 and resid 385 and name C) (segid HEM and resid 1 and name CGA) 7.54 0.12 0.13
 assign (segid 3A4 and resid 385 and name C) (segid HEM and resid 1 and name CHB) 5.71 0.21 0.20
 assign (segid 3A4 and resid 385 and name C) (segid HEM and resid 1 and name CMA) 5.71 0.84 0.84
 assign (segid 3A4 and resid 385 and name C) (segid HEM and resid 1 and name O1A) 6.46 1.27 1.27
 20 assign (segid 3A4 and resid 385 and name C) (segid HEM and resid 1 and name O2A) 1.51 0.01 0.01
 assign (segid 3A4 and resid 385 and name CA) (segid 3A4 and resid 385 and name C) 2.41 0.02 0.02
 assign (segid 3A4 and resid 385 and name CA) (segid 3A4 and resid 385 and name O) 4.82 0.06 0.06
 assign (segid 3A4 and resid 385 and name CA) (segid 3A4 and resid 386 and name C) 3.79 0.01 0.01
 assign (segid 3A4 and resid 385 and name CA) (segid 3A4 and resid 386 and name CA) 2.42 0.01 0.01
 25 assign (segid 3A4 and resid 385 and name CA) (segid 3A4 and resid 386 and name N) 5.09 0.38 0.37
 assign (segid 3A4 and resid 385 and name CA) (segid 3A4 and resid 386 and name O) 7.31 0.10 0.10
 assign (segid 3A4 and resid 385 and name CA) (segid 3A4 and resid 387 and name C) 6.93 0.23 0.23
 assign (segid 3A4 and resid 385 and name CA) (segid 3A4 and resid 387 and name CA) 5.72 0.28 0.28
 assign (segid 3A4 and resid 385 and name CA) (segid 3A4 and resid 387 and name N) 7.07 0.17 0.16
 30 assign (segid 3A4 and resid 385 and name CA) (segid 3A4 and resid 387 and name O) 9.00 0.13 0.12
 assign (segid 3A4 and resid 385 and name CA) (segid 3A4 and resid 388 and name CA) 10.28 0.16 0.15
 assign (segid 3A4 and resid 385 and name CA) (segid 3A4 and resid 388 and name CB) 5.91 0.29 0.28
 assign (segid 3A4 and resid 385 and name CA) (segid 3A4 and resid 389 and name C) 7.09 0.30 0.30
 assign (segid 3A4 and resid 385 and name CA) (segid 3A4 and resid 389 and name CA) 7.16 0.34 0.35
 35 assign (segid 3A4 and resid 385 and name CA) (segid 3A4 and resid 389 and name CB) 7.44 0.24 0.24
 assign (segid 3A4 and resid 385 and name CA) (segid 3A4 and resid 389 and name N) 5.64 0.35 0.34
 assign (segid 3A4 and resid 385 and name CA) (segid 3A4 and resid 390 and name C) 5.55 0.17 0.17
 assign (segid 3A4 and resid 385 and name CA) (segid 3A4 and resid 390 and name CA) 4.77 0.19 0.19
 40 assign (segid 3A4 and resid 385 and name CA) (segid 3A4 and resid 390 and name CB) 5.21 0.22 0.23
 assign (segid 3A4 and resid 385 and name CA) (segid 3A4 and resid 390 and name N) 5.57 0.22 0.22
 assign (segid 3A4 and resid 385 and name CA) (segid 3A4 and resid 390 and name O) 6.73 0.18 0.18
 assign (segid 3A4 and resid 385 and name CA) (segid 3A4 and resid 391 and name C) 7.55 0.12 0.12
 45 assign (segid 3A4 and resid 385 and name CA) (segid 3A4 and resid 391 and name CA) 6.28 0.15 0.15
 assign (segid 3A4 and resid 385 and name CA) (segid 3A4 and resid 391 and name CB) 6.16 0.17 0.17
 assign (segid 3A4 and resid 385 and name CA) (segid 3A4 and resid 391 and name N) 5.20 0.14 0.15
 assign (segid 3A4 and resid 385 and name CA) (segid 3A4 and resid 392 and name CA) 9.90 0.13 0.14
 assign (segid 3A4 and resid 385 and name CA) (segid 3A4 and resid 392 and name CB) 10.88 0.15 0.14
 50 assign (segid 3A4 and resid 385 and name CA) (segid 3A4 and resid 393 and name CA) 11.24 0.16 0.16
 assign (segid 3A4 and resid 385 and name CA) (segid 3A4 and resid 394 and name CA) 9.67 0.18 0.18
 assign (segid 3A4 and resid 385 and name CA) (segid 3A4 and resid 394 and name CB) 8.75 0.24 0.23
 assign (segid 3A4 and resid 385 and name CA) (segid 3A4 and resid 395 and name CA) 13.17 0.27 0.27
 assign (segid 3A4 and resid 385 and name CA) (segid 3A4 and resid 396 and name CA) 15.05 0.16 0.15
 55 assign (segid 3A4 and resid 385 and name CA) (segid 3A4 and resid 396 and name CB) 15.26 0.30 0.30
 assign (segid 3A4 and resid 385 and name CA) (segid 3A4 and resid 397 and name CA) 13.34 0.19 0.19
 assign (segid 3A4 and resid 385 and name CA) (segid 3A4 and resid 397 and name CB) 11.94 0.21 0.22
 assign (segid 3A4 and resid 385 and name CA) (segid 3A4 and resid 398 and name CA) 14.13 0.31 0.30
 assign (segid 3A4 and resid 385 and name CA) (segid 3A4 and resid 398 and name CB) 13.65 0.32 0.31
 60 assign (segid 3A4 and resid 385 and name CA) (segid 3A4 and resid 399 and name CA) 17.55 0.24 0.25
 assign (segid 3A4 and resid 385 and name CA) (segid 3A4 and resid 399 and name CB) 17.97 0.23 0.23
 assign (segid 3A4 and resid 385 and name CA) (segid 3A4 and resid 400 and name CA) 18.43 0.25 0.24
 assign (segid 3A4 and resid 385 and name CA) (segid 3A4 and resid 400 and name CB) 17.88 0.29 0.28
 assign (segid 3A4 and resid 385 and name CA) (segid 3A4 and resid 401 and name CA) 17.60 0.28 0.28
 65 assign (segid 3A4 and resid 385 and name CA) (segid 3A4 and resid 402 and name CB) 19.29 0.27 0.27
 assign (segid 3A4 and resid 385 and name CA) (segid 3A4 and resid 431 and name CA) 14.33 1.45 1.45
 assign (segid 3A4 and resid 385 and name CA) (segid 3A4 and resid 433 and name CA) 15.51 0.28 0.29
 assign (segid 3A4 and resid 385 and name CA) (segid 3A4 and resid 434 and name CA) 17.73 0.64 0.65
 assign (segid 3A4 and resid 385 and name CA) (segid HEM and resid 1 and name C1A) 6.05 0.36 0.37
 70 assign (segid 3A4 and resid 385 and name CA) (segid HEM and resid 1 and name C1B) 7.44 0.21 0.21
 assign (segid 3A4 and resid 385 and name CA) (segid HEM and resid 1 and name C2A) 5.00 0.40 0.40
 assign (segid 3A4 and resid 385 and name CA) (segid HEM and resid 1 and name C3A) 4.78 0.29 0.30
 assign (segid 3A4 and resid 385 and name CA) (segid HEM and resid 1 and name C4A) 5.75 0.22 0.23
 assign (segid 3A4 and resid 385 and name CA) (segid HEM and resid 1 and name CAA) 4.72 0.49 0.50
 75 assign (segid 3A4 and resid 385 and name CA) (segid HEM and resid 1 and name CBA) 4.86 0.54 0.54
 assign (segid 3A4 and resid 385 and name CA) (segid HEM and resid 1 and name CGA) 5.08 0.63 0.64
 assign (segid 3A4 and resid 385 and name CA) (segid HEM and resid 1 and name CHA) 6.93 0.41 0.41
 assign (segid 3A4 and resid 385 and name CA) (segid HEM and resid 1 and name CHB) 6.27 0.20 0.20
 assign (segid 3A4 and resid 385 and name CA) (segid HEM and resid 1 and name CMA) 4.23 0.23 0.22
 80 assign (segid 3A4 and resid 385 and name CA) (segid HEM and resid 1 and name NA) 6.46 0.27 0.27
 assign (segid 3A4 and resid 385 and name CA) (segid HEM and resid 1 and name O1A) 4.97 0.77 0.77
 assign (segid 3A4 and resid 385 and name CA) (segid HEM and resid 1 and name O2A) 5.69 1.09 1.09
 assign (segid 3A4 and resid 385 and name N) (segid 3A4 and resid 385 and name C) 2.43 0.02 0.02
 assign (segid 3A4 and resid 385 and name N) (segid 3A4 and resid 385 and name CA) 1.46 0.02 0.02

	assign (segid 3A4 and resid 385 and name N)	(segid 3A4 and resid 385 and name O)	2.71	0.06	0.06
	assign (segid 3A4 and resid 385 and name N)	(segid 3A4 and resid 386 and name C)	6.00	0.05	0.04
	assign (segid 3A4 and resid 385 and name N)	(segid 3A4 and resid 386 and name CA)	4.85	0.04	0.05
	assign (segid 3A4 and resid 385 and name N)	(segid 3A4 and resid 386 and name N)	3.63	0.02	0.03
5	assign (segid 3A4 and resid 385 and name N)	(segid 3A4 and resid 386 and name O)	6.36	0.27	0.27
	assign (segid 3A4 and resid 385 and name N)	(segid 3A4 and resid 387 and name N)	6.82	0.26	0.25
	assign (segid 3A4 and resid 385 and name N)	(segid 3A4 and resid 389 and name C)	6.72	0.21	0.20
	assign (segid 3A4 and resid 385 and name N)	(segid 3A4 and resid 389 and name O)	6.32	0.24	0.24
	assign (segid 3A4 and resid 385 and name N)	(segid 3A4 and resid 390 and name C)	5.75	0.15	0.14
10	assign (segid 3A4 and resid 385 and name N)	(segid 3A4 and resid 390 and name CA)	5.27	0.18	0.18
	assign (segid 3A4 and resid 385 and name N)	(segid 3A4 and resid 390 and name CB)	5.62	0.28	0.29
	assign (segid 3A4 and resid 385 and name N)	(segid 3A4 and resid 390 and name N)	6.32	0.17	0.17
	assign (segid 3A4 and resid 385 and name N)	(segid 3A4 and resid 390 and name O)	6.96	0.14	0.14
	assign (segid 3A4 and resid 385 and name N)	(segid 3A4 and resid 391 and name C)	7.22	0.08	0.08
15	assign (segid 3A4 and resid 385 and name N)	(segid 3A4 and resid 391 and name CA)	5.96	0.10	0.11
	assign (segid 3A4 and resid 385 and name N)	(segid 3A4 and resid 391 and name CB)	5.50	0.13	0.14
	assign (segid 3A4 and resid 385 and name N)	(segid 3A4 and resid 391 and name N)	5.09	0.10	0.10
	assign (segid 3A4 and resid 385 and name N)	(segid 3A4 and resid 391 and name O)	7.37	0.10	0.10
	assign (segid 3A4 and resid 385 and name N)	(segid HEM and resid 1 and name C1A)	5.84	0.26	0.27
20	assign (segid 3A4 and resid 385 and name N)	(segid HEM and resid 1 and name C1B)	6.40	0.17	0.17
	assign (segid 3A4 and resid 385 and name N)	(segid HEM and resid 1 and name C2A)	4.92	0.30	0.30
	assign (segid 3A4 and resid 385 and name N)	(segid HEM and resid 1 and name C2B)	7.03	0.16	0.15
	assign (segid 3A4 and resid 385 and name N)	(segid HEM and resid 1 and name C3A)	4.39	0.22	0.21
	assign (segid 3A4 and resid 385 and name N)	(segid HEM and resid 1 and name C4A)	5.09	0.17	0.16
25	assign (segid 3A4 and resid 385 and name N)	(segid HEM and resid 1 and name CAA)	5.09	0.38	0.38
	assign (segid 3A4 and resid 385 and name N)	(segid HEM and resid 1 and name CBA)	5.41	0.57	0.56
	assign (segid 3A4 and resid 385 and name N)	(segid HEM and resid 1 and name CGA)	5.96	0.62	0.62
	assign (segid 3A4 and resid 385 and name N)	(segid HEM and resid 1 and name CHA)	6.89	0.30	0.30
	assign (segid 3A4 and resid 385 and name N)	(segid HEM and resid 1 and name CHB)	5.33	0.13	0.14
30	assign (segid 3A4 and resid 385 and name N)	(segid HEM and resid 1 and name CMA)	3.83	0.14	0.14
	assign (segid 3A4 and resid 385 and name N)	(segid HEM and resid 1 and name CMB)	6.80	0.15	0.16
	assign (segid 3A4 and resid 385 and name N)	(segid HEM and resid 1 and name NA)	5.94	0.19	0.19
	assign (segid 3A4 and resid 385 and name N)	(segid HEM and resid 1 and name NB)	7.27	0.16	0.16
	assign (segid 3A4 and resid 385 and name N)	(segid HEM and resid 1 and name O1A)	5.99	0.66	0.66
35	assign (segid 3A4 and resid 385 and name N)	(segid HEM and resid 1 and name O2A)	6.64	1.03	1.03
	assign (segid 3A4 and resid 385 and name O)	(segid 3A4 and resid 386 and name C)	4.17	0.10	0.10
	assign (segid 3A4 and resid 385 and name O)	(segid 3A4 and resid 386 and name N)	2.75	0.05	0.05
	assign (segid 3A4 and resid 385 and name O)	(segid 3A4 and resid 386 and name O)	2.25	0.01	0.01
40	assign (segid 3A4 and resid 385 and name O)	(segid 3A4 and resid 386 and name C)	4.85	0.09	0.10
	assign (segid 3A4 and resid 385 and name O)	(segid 3A4 and resid 387 and name C)	6.88	0.16	0.16
	assign (segid 3A4 and resid 385 and name O)	(segid 3A4 and resid 387 and name CA)	6.32	0.15	0.14
	assign (segid 3A4 and resid 385 and name O)	(segid 3A4 and resid 387 and name N)	4.91	0.16	0.15
	assign (segid 3A4 and resid 385 and name O)	(segid 3A4 and resid 387 and name O)	6.53	0.17	0.17
45	assign (segid 3A4 and resid 385 and name O)	(segid 3A4 and resid 389 and name C)	6.81	0.25	0.25
	assign (segid 3A4 and resid 385 and name O)	(segid 3A4 and resid 389 and name O)	6.89	0.30	0.29
	assign (segid 3A4 and resid 385 and name O)	(segid 3A4 and resid 390 and name C)	6.12	0.14	0.15
	assign (segid 3A4 and resid 385 and name O)	(segid 3A4 and resid 390 and name CA)	5.14	0.20	0.19
	assign (segid 3A4 and resid 385 and name O)	(segid 3A4 and resid 390 and name CB)	4.86	0.32	0.32
50	assign (segid 3A4 and resid 385 and name O)	(segid 3A4 and resid 390 and name N)	6.05	0.20	0.21
	assign (segid 3A4 and resid 385 and name O)	(segid 3A4 and resid 390 and name O)	7.28	0.16	0.17
	assign (segid 3A4 and resid 385 and name O)	(segid 3A4 and resid 391 and name CA)	7.14	0.09	0.09
	assign (segid 3A4 and resid 385 and name O)	(segid 3A4 and resid 391 and name CB)	7.04	0.12	0.11
	assign (segid 3A4 and resid 385 and name O)	(segid 3A4 and resid 391 and name N)	5.93	0.08	0.09
55	assign (segid 3A4 and resid 385 and name O)	(segid HEM and resid 1 and name C2A)	7.11	0.27	0.27
	assign (segid 3A4 and resid 385 and name O)	(segid HEM and resid 1 and name C3A)	6.86	0.15	0.16
	assign (segid 3A4 and resid 385 and name O)	(segid HEM and resid 1 and name C4A)	7.58	0.06	0.06
	assign (segid 3A4 and resid 385 and name O)	(segid HEM and resid 1 and name CBA)	7.04	0.67	0.68
	assign (segid 3A4 and resid 385 and name O)	(segid HEM and resid 1 and name CGA)	7.14	0.74	0.74
	assign (segid 3A4 and resid 385 and name O)	(segid HEM and resid 1 and name CMA)	6.39	0.13	0.13
60	assign (segid 3A4 and resid 386 and name C)	(segid 3A4 and resid 386 and name O)	1.23	0.00	0.00
	assign (segid 3A4 and resid 386 and name C)	(segid 3A4 and resid 387 and name C)	3.23	0.10	0.10
	assign (segid 3A4 and resid 386 and name C)	(segid 3A4 and resid 387 and name CA)	2.40	0.02	0.02
	assign (segid 3A4 and resid 386 and name C)	(segid 3A4 and resid 387 and name N)	1.33	0.01	0.00
	assign (segid 3A4 and resid 386 and name C)	(segid 3A4 and resid 387 and name O)	3.46	0.18	0.17
65	assign (segid 3A4 and resid 386 and name C)	(segid 3A4 and resid 388 and name C)	5.64	0.26	0.26
	assign (segid 3A4 and resid 386 and name C)	(segid 3A4 and resid 388 and name CA)	5.45	0.15	0.15
	assign (segid 3A4 and resid 386 and name C)	(segid 3A4 and resid 388 and name CB)	6.64	0.11	0.11
	assign (segid 3A4 and resid 386 and name C)	(segid 3A4 and resid 388 and name N)	4.26	0.14	0.13
	assign (segid 3A4 and resid 386 and name C)	(segid 3A4 and resid 388 and name O)	6.65	0.27	0.27
70	assign (segid 3A4 and resid 386 and name C)	(segid 3A4 and resid 389 and name C)	5.25	0.39	0.39
	assign (segid 3A4 and resid 386 and name C)	(segid 3A4 and resid 389 and name CA)	5.69	0.39	0.40
	assign (segid 3A4 and resid 386 and name C)	(segid 3A4 and resid 389 and name CB)	6.11	0.45	0.45
	assign (segid 3A4 and resid 386 and name C)	(segid 3A4 and resid 389 and name N)	5.03	0.34	0.33
	assign (segid 3A4 and resid 386 and name C)	(segid 3A4 and resid 389 and name O)	5.98	0.45	0.44
75	assign (segid 3A4 and resid 386 and name C)	(segid 3A4 and resid 390 and name C)	6.16	0.23	0.24
	assign (segid 3A4 and resid 386 and name C)	(segid 3A4 and resid 390 and name CA)	4.66	0.25	0.25
	assign (segid 3A4 and resid 386 and name C)	(segid 3A4 and resid 390 and name CB)	4.37	0.31	0.31
	assign (segid 3A4 and resid 386 and name C)	(segid 3A4 and resid 390 and name N)	4.53	0.29	0.29
	assign (segid 3A4 and resid 386 and name C)	(segid 3A4 and resid 390 and name O)	6.93	0.30	0.30
80	assign (segid 3A4 and resid 386 and name C)	(segid 3A4 and resid 391 and name N)	6.79	0.16	0.16
	assign (segid 3A4 and resid 386 and name CA)	(segid 3A4 and resid 386 and name C)	1.52	0.01	0.02
	assign (segid 3A4 and resid 386 and name CA)	(segid 3A4 and resid 386 and name O)	2.39	0.02	0.02
	assign (segid 3A4 and resid 386 and name CA)	(segid 3A4 and resid 387 and name C)	4.58	0.06	0.06

	assign (segid 3A4 and resid 386 and name CA) (segid 3A4 and resid 387 and name CA)	3.79	0.03	0.02
	assign (segid 3A4 and resid 386 and name CA) (segid 3A4 and resid 387 and name N)	2.42	0.02	0.02
	assign (segid 3A4 and resid 386 and name CA) (segid 3A4 and resid 387 and name O)	4.57	0.13	0.12
	assign (segid 3A4 and resid 386 and name CA) (segid 3A4 and resid 388 and name C)	6.84	0.19	0.20
5	assign (segid 3A4 and resid 386 and name CA) (segid 3A4 and resid 388 and name CA)	6.81	0.10	0.10
	assign (segid 3A4 and resid 386 and name CA) (segid 3A4 and resid 388 and name CB)	8.07	0.08	0.07
	assign (segid 3A4 and resid 386 and name CA) (segid 3A4 and resid 388 and name N)	5.68	0.09	0.10
	assign (segid 3A4 and resid 386 and name CA) (segid 3A4 and resid 389 and name C)	5.84	0.33	0.34
	assign (segid 3A4 and resid 386 and name CA) (segid 3A4 and resid 389 and name CA)	6.58	0.33	0.34
10	assign (segid 3A4 and resid 386 and name CA) (segid 3A4 and resid 389 and name CB)	6.97	0.44	0.43
	assign (segid 3A4 and resid 386 and name CA) (segid 3A4 and resid 389 and name N)	6.16	0.27	0.28
	assign (segid 3A4 and resid 386 and name CA) (segid 3A4 and resid 389 and name O)	6.33	0.42	0.43
	assign (segid 3A4 and resid 386 and name CA) (segid 3A4 and resid 390 and name C)	6.20	0.17	0.16
	assign (segid 3A4 and resid 386 and name CA) (segid 3A4 and resid 390 and name CA)	4.78	0.19	0.19
	assign (segid 3A4 and resid 386 and name CA) (segid 3A4 and resid 390 and name CB)	4.44	0.28	0.27
15	assign (segid 3A4 and resid 386 and name CA) (segid 3A4 and resid 390 and name N)	5.08	0.22	0.21
	assign (segid 3A4 and resid 386 and name CA) (segid 3A4 and resid 390 and name O)	7.14	0.20	0.20
	assign (segid 3A4 and resid 386 and name CA) (segid 3A4 and resid 391 and name CA)	7.97	0.12	0.12
	assign (segid 3A4 and resid 386 and name CA) (segid 3A4 and resid 391 and name CB)	8.36	0.10	0.10
20	assign (segid 3A4 and resid 386 and name CA) (segid 3A4 and resid 391 and name N)	6.56	0.13	0.13
	assign (segid 3A4 and resid 386 and name CA) (segid 3A4 and resid 392 and name CA)	10.85	0.21	0.21
	assign (segid 3A4 and resid 386 and name CA) (segid 3A4 and resid 392 and name CB)	11.79	0.20	0.19
	assign (segid 3A4 and resid 386 and name CA) (segid 3A4 and resid 393 and name CA)	13.00	0.22	0.22
	assign (segid 3A4 and resid 386 and name CA) (segid 3A4 and resid 394 and name CA)	11.34	0.45	0.46
25	assign (segid 3A4 and resid 386 and name CA) (segid 3A4 and resid 394 and name CB)	10.10	0.50	0.51
	assign (segid 3A4 and resid 386 and name CA) (segid 3A4 and resid 395 and name CA)	14.31	0.62	0.63
	assign (segid 3A4 and resid 386 and name CA) (segid 3A4 and resid 396 and name CA)	16.80	0.41	0.42
	assign (segid 3A4 and resid 386 and name CA) (segid 3A4 and resid 396 and name CB)	17.07	0.36	0.36
	assign (segid 3A4 and resid 386 and name CA) (segid 3A4 and resid 397 and name CA)	15.74	0.38	0.37
30	assign (segid 3A4 and resid 386 and name CA) (segid 3A4 and resid 397 and name CB)	14.48	0.36	0.36
	assign (segid 3A4 and resid 386 and name CA) (segid 3A4 and resid 398 and name CA)	16.09	0.56	0.57
	assign (segid 3A4 and resid 386 and name CA) (segid 3A4 and resid 398 and name CB)	15.33	0.60	0.61
	assign (segid 3A4 and resid 386 and name CA) (segid 3A4 and resid 433 and name CA)	19.18	0.32	0.31
	assign (segid 3A4 and resid 386 and name CA) (segid HEM and resid 1 and name CBA)	7.28	0.63	0.64
35	assign (segid 3A4 and resid 386 and name CA) (segid HEM and resid 1 and name CB)	6.85	0.75	0.75
	assign (segid 3A4 and resid 386 and name N) (segid 3A4 and resid 386 and name C)	2.44	0.05	0.06
	assign (segid 3A4 and resid 386 and name N) (segid 3A4 and resid 386 and name O)	1.46	0.00	0.00
	assign (segid 3A4 and resid 386 and name N) (segid 3A4 and resid 387 and name C)	2.90	0.28	0.28
	assign (segid 3A4 and resid 386 and name N) (segid 3A4 and resid 387 and name N)	5.25	0.09	0.10
40	assign (segid 3A4 and resid 386 and name N) (segid 3A4 and resid 387 and name O)	4.68	0.19	0.19
	assign (segid 3A4 and resid 386 and name N) (segid 3A4 and resid 388 and name C)	3.42	0.25	0.25
	assign (segid 3A4 and resid 386 and name N) (segid 3A4 and resid 388 and name CA)	5.17	0.14	0.14
	assign (segid 3A4 and resid 386 and name N) (segid 3A4 and resid 388 and name CB)	6.97	0.20	0.21
	assign (segid 3A4 and resid 386 and name N) (segid 3A4 and resid 388 and name N)	7.23	0.10	0.10
45	assign (segid 3A4 and resid 386 and name N) (segid 3A4 and resid 388 and name O)	6.24	0.05	0.06
	assign (segid 3A4 and resid 386 and name N) (segid 3A4 and resid 389 and name C)	5.30	0.34	0.33
	assign (segid 3A4 and resid 386 and name N) (segid 3A4 and resid 389 and name CA)	6.21	0.33	0.33
	assign (segid 3A4 and resid 386 and name N) (segid 3A4 and resid 389 and name CB)	6.45	0.39	0.39
	assign (segid 3A4 and resid 386 and name N) (segid 3A4 and resid 389 and name N)	6.11	0.26	0.25
50	assign (segid 3A4 and resid 386 and name N) (segid 3A4 and resid 389 and name O)	5.53	0.44	0.44
	assign (segid 3A4 and resid 386 and name N) (segid 3A4 and resid 390 and name C)	5.56	0.16	0.17
	assign (segid 3A4 and resid 386 and name N) (segid 3A4 and resid 390 and name CA)	4.27	0.20	0.20
	assign (segid 3A4 and resid 386 and name N) (segid 3A4 and resid 390 and name CB)	4.33	0.23	0.24
	assign (segid 3A4 and resid 386 and name N) (segid 3A4 and resid 390 and name N)	4.71	0.23	0.24
55	assign (segid 3A4 and resid 386 and name N) (segid 3A4 and resid 390 and name O)	6.61	0.19	0.20
	assign (segid 3A4 and resid 386 and name N) (segid 3A4 and resid 391 and name CA)	7.10	0.09	0.09
	assign (segid 3A4 and resid 386 and name N) (segid 3A4 and resid 391 and name CB)	7.40	0.07	0.07
	assign (segid 3A4 and resid 386 and name N) (segid 3A4 and resid 391 and name N)	5.75	0.11	0.11
	assign (segid 3A4 and resid 386 and name N) (segid HEM and resid 1 and name C2A)	6.67	0.38	0.39
60	assign (segid 3A4 and resid 386 and name N) (segid HEM and resid 1 and name C3A)	6.81	0.26	0.27
	assign (segid 3A4 and resid 386 and name N) (segid HEM and resid 1 and name C4A)	6.06	0.54	0.54
	assign (segid 3A4 and resid 386 and name N) (segid HEM and resid 1 and name CBA)	5.98	0.60	0.61
	assign (segid 3A4 and resid 386 and name N) (segid HEM and resid 1 and name CGA)	5.67	0.74	0.74
	assign (segid 3A4 and resid 386 and name N) (segid HEM and resid 1 and name CMA)	6.45	0.23	0.23
65	assign (segid 3A4 and resid 386 and name N) (segid HEM and resid 1 and name O1A)	5.29	0.88	0.88
	assign (segid 3A4 and resid 386 and name N) (segid HEM and resid 1 and name O2A)	6.05	1.32	1.33
	assign (segid 3A4 and resid 386 and name O) (segid 3A4 and resid 387 and name C)	3.32	0.19	0.20
	assign (segid 3A4 and resid 386 and name O) (segid 3A4 and resid 387 and name CA)	2.73	0.04	0.04
	assign (segid 3A4 and resid 386 and name O) (segid 3A4 and resid 387 and name N)	2.25	0.02	0.01
70	assign (segid 3A4 and resid 386 and name O) (segid 3A4 and resid 387 and name O)	3.67	0.37	0.36
	assign (segid 3A4 and resid 386 and name O) (segid 3A4 and resid 388 and name C)	5.35	0.55	0.55
	assign (segid 3A4 and resid 386 and name O) (segid 3A4 and resid 388 and name CA)	5.21	0.31	0.32
	assign (segid 3A4 and resid 386 and name O) (segid 3A4 and resid 388 and name CB)	6.26	0.23	0.23
	assign (segid 3A4 and resid 386 and name O) (segid 3A4 and resid 388 and name N)	4.08	0.26	0.27
75	assign (segid 3A4 and resid 386 and name O) (segid 3A4 and resid 388 and name O)	6.41	0.56	0.56
	assign (segid 3A4 and resid 386 and name O) (segid 3A4 and resid 389 and name C)	5.01	0.84	0.84
	assign (segid 3A4 and resid 386 and name O) (segid 3A4 and resid 389 and name CA)	5.26	0.85	0.86
	assign (segid 3A4 and resid 386 and name O) (segid 3A4 and resid 389 and name CB)	5.51	0.96	0.96
	assign (segid 3A4 and resid 386 and name O) (segid 3A4 and resid 389 and name N)	4.61	0.71	0.72
80	assign (segid 3A4 and resid 386 and name O) (segid 3A4 and resid 389 and name O)	5.75	0.89	0.88
	assign (segid 3A4 and resid 386 and name O) (segid 3A4 and resid 390 and name C)	6.35	0.50	0.50
	assign (segid 3A4 and resid 386 and name O) (segid 3A4 and resid 390 and name CA)	4.89	0.51	0.51
	assign (segid 3A4 and resid 386 and name O) (segid 3A4 and resid 390 and name CB)	4.86	0.42	0.42

	assign (segid 3A4 and resid 386 and name O) (segid 3A4 and resid 390 and name N)	4.52	0.66	0.65
	assign (segid 3A4 and resid 386 and name O) (segid 3A4 and resid 390 and name O)	7.06	0.60	0.60
	assign (segid 3A4 and resid 386 and name O) (segid 3A4 and resid 391 and name N)	7.01	0.39	0.40
	assign (segid 3A4 and resid 387 and name C) (segid 3A4 and resid 387 and name O)	1.24	0.01	0.01
5	assign (segid 3A4 and resid 387 and name C) (segid 3A4 and resid 388 and name C)	3.13	0.04	0.03
	assign (segid 3A4 and resid 387 and name C) (segid 3A4 and resid 388 and name CA)	2.44	0.01	0.01
	assign (segid 3A4 and resid 387 and name C) (segid 3A4 and resid 388 and name CB)	3.71	0.04	0.03
	assign (segid 3A4 and resid 387 and name C) (segid 3A4 and resid 388 and name N)	1.34	0.01	0.01
	assign (segid 3A4 and resid 387 and name C) (segid 3A4 and resid 388 and name O)	4.14	0.10	0.11
10	assign (segid 3A4 and resid 387 and name C) (segid 3A4 and resid 389 and name C)	4.63	0.09	0.09
	assign (segid 3A4 and resid 387 and name C) (segid 3A4 and resid 389 and name CA)	4.46	0.07	0.06
	assign (segid 3A4 and resid 387 and name C) (segid 3A4 and resid 389 and name CB)	5.32	0.13	0.14
	assign (segid 3A4 and resid 387 and name C) (segid 3A4 and resid 389 and name N)	3.21	0.08	0.09
	assign (segid 3A4 and resid 387 and name C) (segid 3A4 and resid 389 and name O)	5.78	0.13	0.14
15	assign (segid 3A4 and resid 387 and name C) (segid 3A4 and resid 390 and name C)	6.04	0.14	0.14
	assign (segid 3A4 and resid 387 and name C) (segid 3A4 and resid 390 and name CA)	4.74	0.12	0.12
	assign (segid 3A4 and resid 387 and name C) (segid 3A4 and resid 390 and name CB)	4.39	0.13	0.13
	assign (segid 3A4 and resid 387 and name C) (segid 3A4 and resid 390 and name N)	3.92	0.09	0.08
	assign (segid 3A4 and resid 387 and name C) (segid 3A4 and resid 390 and name O)	6.27	0.21	0.21
20	assign (segid 3A4 and resid 387 and name C) (segid 3A4 and resid 391 and name N)	7.13	0.13	0.12
	assign (segid 3A4 and resid 387 and name C) (segid 3A4 and resid 387 and name C)	1.51	0.00	0.00
	assign (segid 3A4 and resid 387 and name CA) (segid 3A4 and resid 387 and name O)	2.40	0.01	0.01
	assign (segid 3A4 and resid 387 and name CA) (segid 3A4 and resid 388 and name C)	4.48	0.05	0.05
	assign (segid 3A4 and resid 387 and name CA) (segid 3A4 and resid 388 and name CA)	3.78	0.01	0.01
25	assign (segid 3A4 and resid 387 and name CA) (segid 3A4 and resid 388 and name CB)	4.82	0.03	0.03
	assign (segid 3A4 and resid 387 and name CA) (segid 3A4 and resid 388 and name N)	2.40	0.01	0.01
	assign (segid 3A4 and resid 387 and name CA) (segid 3A4 and resid 388 and name O)	5.56	0.07	0.07
	assign (segid 3A4 and resid 387 and name CA) (segid 3A4 and resid 389 and name C)	5.47	0.26	0.26
	assign (segid 3A4 and resid 387 and name CA) (segid 3A4 and resid 389 and name CA)	5.42	0.22	0.22
30	assign (segid 3A4 and resid 387 and name CA) (segid 3A4 and resid 389 and name CB)	6.02	0.31	0.30
	assign (segid 3A4 and resid 387 and name CA) (segid 3A4 and resid 389 and name N)	4.29	0.18	0.18
	assign (segid 3A4 and resid 387 and name CA) (segid 3A4 and resid 389 and name O)	6.50	0.33	0.34
	assign (segid 3A4 and resid 387 and name CA) (segid 3A4 and resid 390 and name C)	6.82	0.25	0.26
	assign (segid 3A4 and resid 387 and name CA) (segid 3A4 and resid 390 and name CA)	5.38	0.26	0.26
35	assign (segid 3A4 and resid 387 and name CA) (segid 3A4 and resid 390 and name CB)	4.98	0.23	0.23
	assign (segid 3A4 and resid 387 and name CA) (segid 3A4 and resid 390 and name N)	4.77	0.22	0.23
	assign (segid 3A4 and resid 387 and name CA) (segid 3A4 and resid 390 and name O)	7.25	0.28	0.29
	assign (segid 3A4 and resid 387 and name CA) (segid 3A4 and resid 391 and name CA)	9.15	0.25	0.25
	assign (segid 3A4 and resid 387 and name CA) (segid 3A4 and resid 391 and name CB)	10.06	0.22	0.23
40	assign (segid 3A4 and resid 387 and name CA) (segid 3A4 and resid 392 and name CA)	11.10	0.41	0.41
	assign (segid 3A4 and resid 387 and name CA) (segid 3A4 and resid 392 and name CB)	11.71	0.39	0.39
	assign (segid 3A4 and resid 387 and name CA) (segid 3A4 and resid 393 and name CA)	14.06	0.40	0.40
	assign (segid 3A4 and resid 387 and name CA) (segid 3A4 and resid 394 and name CA)	13.05	0.54	0.55
	assign (segid 3A4 and resid 387 and name CA) (segid 3A4 and resid 394 and name CB)	11.82	0.58	0.58
45	assign (segid 3A4 and resid 387 and name CA) (segid 3A4 and resid 395 and name CA)	15.67	0.67	0.68
	assign (segid 3A4 and resid 387 and name CA) (segid 3A4 and resid 396 and name CA)	18.24	0.57	0.57
	assign (segid 3A4 and resid 387 and name CA) (segid 3A4 and resid 396 and name CB)	18.34	0.58	0.58
	assign (segid 3A4 and resid 387 and name CA) (segid 3A4 and resid 397 and name CA)	17.82	0.42	0.41
	assign (segid 3A4 and resid 387 and name CA) (segid 3A4 and resid 397 and name CB)	16.67	0.38	0.37
50	assign (segid 3A4 and resid 387 and name CA) (segid 3A4 and resid 398 and name CA)	18.39	0.50	0.50
	assign (segid 3A4 and resid 387 and name CA) (segid 3A4 and resid 398 and name CB)	17.58	0.55	0.56
	assign (segid 3A4 and resid 387 and name N) (segid 3A4 and resid 387 and name C)	2.48	0.01	0.02
	assign (segid 3A4 and resid 387 and name N) (segid 3A4 and resid 387 and name CA)	1.46	0.02	0.02
	assign (segid 3A4 and resid 387 and name N) (segid 3A4 and resid 387 and name O)	2.82	0.06	0.05
55	assign (segid 3A4 and resid 387 and name N) (segid 3A4 and resid 388 and name C)	5.27	0.03	0.04
	assign (segid 3A4 and resid 387 and name N) (segid 3A4 and resid 388 and name CA)	4.88	0.02	0.02
	assign (segid 3A4 and resid 387 and name N) (segid 3A4 and resid 388 and name CB)	6.08	0.03	0.04
	assign (segid 3A4 and resid 387 and name N) (segid 3A4 and resid 388 and name N)	3.62	0.02	0.02
	assign (segid 3A4 and resid 387 and name N) (segid 3A4 and resid 388 and name O)	6.27	0.08	0.09
60	assign (segid 3A4 and resid 387 and name N) (segid 3A4 and resid 389 and name C)	5.41	0.27	0.28
	assign (segid 3A4 and resid 387 and name N) (segid 3A4 and resid 389 and name CA)	5.74	0.21	0.22
	assign (segid 3A4 and resid 387 and name N) (segid 3A4 and resid 389 and name CB)	6.33	0.30	0.29
	assign (segid 3A4 and resid 387 and name N) (segid 3A4 and resid 389 and name N)	4.89	0.17	0.16
	assign (segid 3A4 and resid 387 and name N) (segid 3A4 and resid 389 and name O)	6.28	0.08	0.07
65	assign (segid 3A4 and resid 387 and name N) (segid 3A4 and resid 390 and name C)	6.32	0.28	0.27
	assign (segid 3A4 and resid 387 and name N) (segid 3A4 and resid 390 and name CA)	4.82	0.28	0.28
	assign (segid 3A4 and resid 387 and name N) (segid 3A4 and resid 390 and name CB)	4.32	0.26	0.27
	assign (segid 3A4 and resid 387 and name N) (segid 3A4 and resid 390 and name N)	4.59	0.22	0.22
	assign (segid 3A4 and resid 387 and name N) (segid 3A4 and resid 390 and name O)	6.95	0.29	0.29
70	assign (segid 3A4 and resid 387 and name N) (segid 3A4 and resid 391 and name N)	7.08	0.28	0.29
	assign (segid 3A4 and resid 387 and name O) (segid 3A4 and resid 388 and name C)	3.18	0.17	0.17
	assign (segid 3A4 and resid 387 and name O) (segid 3A4 and resid 388 and name CA)	2.80	0.03	0.03
	assign (segid 3A4 and resid 387 and name O) (segid 3A4 and resid 388 and name CB)	4.25	0.07	0.08
	assign (segid 3A4 and resid 387 and name O) (segid 3A4 and resid 388 and name N)	2.27	0.02	0.03
75	assign (segid 3A4 and resid 387 and name O) (segid 3A4 and resid 388 and name O)	3.93	0.27	0.27
	assign (segid 3A4 and resid 387 and name O) (segid 3A4 and resid 389 and name C)	1.33	0.21	0.20
	assign (segid 3A4 and resid 387 and name O) (segid 3A4 and resid 389 and name CA)	4.44	0.19	0.20
	assign (segid 3A4 and resid 387 and name O) (segid 3A4 and resid 389 and name CB)	5.55	0.16	0.17
	assign (segid 3A4 and resid 387 and name O) (segid 3A4 and resid 389 and name N)	3.40	0.16	0.16
80	assign (segid 3A4 and resid 387 and name O) (segid 3A4 and resid 389 and name O)	5.46	0.20	0.19
	assign (segid 3A4 and resid 387 and name O) (segid 3A4 and resid 390 and name C)	5.22	0.20	0.21
	assign (segid 3A4 and resid 387 and name O) (segid 3A4 and resid 390 and name CA)	4.00	0.16	0.16
	assign (segid 3A4 and resid 387 and name O) (segid 3A4 and resid 390 and name CB)	3.43	0.14	0.13

	assign (segid 3A4 and resid 387 and name O)	(segid 3A4 and resid 390 and name N)	3.36	0.20	0.20
	assign (segid 3A4 and resid 387 and name O)	(segid 3A4 and resid 390 and name O)	5.42	0.28	0.29
	assign (segid 3A4 and resid 387 and name O)	(segid 3A4 and resid 391 and name CA)	7.59	0.20	0.21
	assign (segid 3A4 and resid 387 and name O)	(segid 3A4 and resid 391 and name N)	6.31	0.18	0.18
	assign (segid 3A4 and resid 388 and name C)	(segid 3A4 and resid 388 and name CB)	2.50	0.03	0.04
5	assign (segid 3A4 and resid 388 and name C)	(segid 3A4 and resid 388 and name O)	1.23	0.01	0.01
	assign (segid 3A4 and resid 388 and name C)	(segid 3A4 and resid 389 and name C)	3.35	0.04	0.04
	assign (segid 3A4 and resid 388 and name C)	(segid 3A4 and resid 389 and name CA)	2.44	0.02	0.03
	assign (segid 3A4 and resid 388 and name C)	(segid 3A4 and resid 389 and name CB)	3.60	0.05	0.05
	assign (segid 3A4 and resid 388 and name C)	(segid 3A4 and resid 389 and name N)	1.33	0.01	0.02
10	assign (segid 3A4 and resid 388 and name C)	(segid 3A4 and resid 389 and name O)	4.52	0.05	0.05
	assign (segid 3A4 and resid 388 and name C)	(segid 3A4 and resid 390 and name C)	5.42	0.09	0.09
	assign (segid 3A4 and resid 388 and name C)	(segid 3A4 and resid 390 and name CA)	4.70	0.06	0.07
	assign (segid 3A4 and resid 388 and name C)	(segid 3A4 and resid 390 and name CB)	5.03	0.07	0.07
	assign (segid 3A4 and resid 388 and name C)	(segid 3A4 and resid 390 and name N)	3.33	0.05	0.06
15	assign (segid 3A4 and resid 388 and name C)	(segid 3A4 and resid 391 and name CA)	5.12	0.18	0.17
	assign (segid 3A4 and resid 388 and name C)	(segid 3A4 and resid 391 and name O)	7.67	0.09	0.10
	assign (segid 3A4 and resid 388 and name C)	(segid 3A4 and resid 391 and name N)	6.68	0.08	0.08
	assign (segid 3A4 and resid 388 and name C)	(segid HEM and resid 1 and name CBD)	6.42	0.29	0.28
	assign (segid 3A4 and resid 388 and name C)	(segid HEM and resid 1 and name CGD)	5.58	0.30	0.31
20	assign (segid 3A4 and resid 388 and name C)	(segid HEM and resid 1 and name O1D)	5.17	0.27	0.26
	assign (segid 3A4 and resid 388 and name C)	(segid HEM and resid 1 and name O2D)	5.69	0.64	0.64
	assign (segid 3A4 and resid 388 and name CA)	(segid 3A4 and resid 388 and name C)	1.52	0.01	0.01
	assign (segid 3A4 and resid 388 and name CA)	(segid 3A4 and resid 388 and name CB)	1.54	0.02	0.02
	assign (segid 3A4 and resid 388 and name CA)	(segid 3A4 and resid 388 and name O)	2.39	0.01	0.02
25	assign (segid 3A4 and resid 388 and name CA)	(segid 3A4 and resid 389 and name C)	4.62	0.05	0.05
	assign (segid 3A4 and resid 388 and name CA)	(segid 3A4 and resid 389 and name CA)	3.81	0.02	0.01
	assign (segid 3A4 and resid 388 and name CA)	(segid 3A4 and resid 389 and name CB)	4.77	0.04	0.05
	assign (segid 3A4 and resid 388 and name CA)	(segid 3A4 and resid 389 and name N)	2.43	0.03	0.03
	assign (segid 3A4 and resid 388 and name CA)	(segid 3A4 and resid 389 and name O)	5.83	0.04	0.04
30	assign (segid 3A4 and resid 388 and name CA)	(segid 3A4 and resid 390 and name C)	6.50	0.13	0.12
	assign (segid 3A4 and resid 388 and name CA)	(segid 3A4 and resid 390 and name CA)	5.58	0.09	0.09
	assign (segid 3A4 and resid 388 and name CA)	(segid 3A4 and resid 390 and name CB)	5.57	0.10	0.09
	assign (segid 3A4 and resid 388 and name CA)	(segid 3A4 and resid 390 and name N)	4.34	0.07	0.07
	assign (segid 3A4 and resid 388 and name CA)	(segid 3A4 and resid 390 and name O)	6.29	0.22	0.22
35	assign (segid 3A4 and resid 388 and name CA)	(segid 3A4 and resid 391 and name CA)	8.83	0.15	0.15
	assign (segid 3A4 and resid 388 and name CA)	(segid 3A4 and resid 391 and name CB)	10.13	0.12	0.13
	assign (segid 3A4 and resid 388 and name CA)	(segid 3A4 and resid 391 and name N)	7.75	0.12	0.11
	assign (segid 3A4 and resid 388 and name CA)	(segid 3A4 and resid 392 and name CA)	9.69	0.47	0.46
	assign (segid 3A4 and resid 388 and name CA)	(segid 3A4 and resid 392 and name CB)	9.86	0.46	0.46
40	assign (segid 3A4 and resid 388 and name CA)	(segid 3A4 and resid 393 and name CA)	13.20	0.42	0.41
	assign (segid 3A4 and resid 388 and name CA)	(segid 3A4 and resid 394 and name CA)	13.16	0.50	0.51
	assign (segid 3A4 and resid 388 and name CA)	(segid 3A4 and resid 394 and name CB)	12.15	0.55	0.55
	assign (segid 3A4 and resid 388 and name CA)	(segid 3A4 and resid 395 and name CA)	15.55	0.64	0.63
	assign (segid 3A4 and resid 388 and name CA)	(segid 3A4 and resid 396 and name CA)	17.76	0.58	0.58
45	assign (segid 3A4 and resid 388 and name CA)	(segid 3A4 and resid 396 and name CB)	17.59	0.62	0.62
	assign (segid 3A4 and resid 388 and name CA)	(segid 3A4 and resid 397 and name CA)	17.94	0.39	0.39
	assign (segid 3A4 and resid 388 and name CA)	(segid 3A4 and resid 397 and name CB)	16.90	0.33	0.34
	assign (segid 3A4 and resid 388 and name CA)	(segid 3A4 and resid 398 and name CA)	19.03	0.46	0.46
	assign (segid 3A4 and resid 388 and name CA)	(segid 3A4 and resid 398 and name CB)	18.34	0.52	0.52
50	assign (segid 3A4 and resid 388 and name CA)	(segid HEM and resid 1 and name CGD)	7.06	0.31	0.32
	assign (segid 3A4 and resid 388 and name CA)	(segid HEM and resid 1 and name O1D)	6.60	0.28	0.28
	assign (segid 3A4 and resid 388 and name CB)	(segid 3A4 and resid 389 and name C)	5.74	0.09	0.09
	assign (segid 3A4 and resid 388 and name CB)	(segid 3A4 and resid 389 and name CB)	4.62	0.12	0.12
	assign (segid 3A4 and resid 388 and name CB)	(segid 3A4 and resid 389 and name N)	5.30	0.14	0.14
55	assign (segid 3A4 and resid 388 and name CB)	(segid 3A4 and resid 389 and name O)	3.34	0.13	0.13
	assign (segid 3A4 and resid 388 and name CB)	(segid 3A4 and resid 390 and name CA)	6.89	0.11	0.10
	assign (segid 3A4 and resid 388 and name CB)	(segid 3A4 and resid 390 and name CB)	7.00	0.09	0.09
	assign (segid 3A4 and resid 388 and name CB)	(segid 3A4 and resid 390 and name N)	7.07	0.07	0.08
	assign (segid 3A4 and resid 388 and name CB)	(segid 3A4 and resid 390 and name O)	5.69	0.08	0.08
60	assign (segid 3A4 and resid 388 and name CB)	(segid 3A4 and resid 391 and name CA)	7.55	0.18	0.19
	assign (segid 3A4 and resid 388 and name CB)	(segid 3A4 and resid 391 and name CB)	10.11	0.10	0.10
	assign (segid 3A4 and resid 388 and name CB)	(segid 3A4 and resid 392 and name CA)	11.46	0.08	0.08
	assign (segid 3A4 and resid 388 and name CB)	(segid 3A4 and resid 392 and name CB)	10.76	0.45	0.46
	assign (segid 3A4 and resid 388 and name CB)	(segid 3A4 and resid 392 and name N)	10.77	0.47	0.46
65	assign (segid 3A4 and resid 388 and name CB)	(segid 3A4 and resid 393 and name CA)	14.36	0.40	0.40
	assign (segid 3A4 and resid 388 and name CB)	(segid 3A4 and resid 394 and name CA)	14.55	0.49	0.48
	assign (segid 3A4 and resid 388 and name CB)	(segid 3A4 and resid 394 and name CB)	13.57	0.54	0.54
	assign (segid 3A4 and resid 388 and name CB)	(segid 3A4 and resid 395 and name CA)	16.87	0.65	0.65
	assign (segid 3A4 and resid 388 and name CB)	(segid 3A4 and resid 396 and name CA)	19.00	0.59	0.58
70	assign (segid 3A4 and resid 388 and name CB)	(segid 3A4 and resid 396 and name CB)	18.76	0.63	0.63
	assign (segid 3A4 and resid 388 and name CB)	(segid 3A4 and resid 397 and name CA)	19.27	0.36	0.37
	assign (segid 3A4 and resid 388 and name CB)	(segid 3A4 and resid 397 and name CB)	18.25	0.31	0.31
	assign (segid 3A4 and resid 388 and name CB)	(segid HEM and resid 1 and name O1D)	6.99	0.31	0.32
	assign (segid 3A4 and resid 388 and name N)	(segid 3A4 and resid 388 and name C)	2.46	0.07	0.07
75	assign (segid 3A4 and resid 388 and name N)	(segid 3A4 and resid 388 and name CA)	1.46	0.01	0.01
	assign (segid 3A4 and resid 388 and name N)	(segid 3A4 and resid 388 and name CB)	2.47	0.01	0.01
	assign (segid 3A4 and resid 388 and name N)	(segid 3A4 and resid 388 and name O)	3.57	0.05	0.06
	assign (segid 3A4 and resid 388 and name N)	(segid 3A4 and resid 389 and name C)	4.75	0.17	0.17
	assign (segid 3A4 and resid 388 and name N)	(segid 3A4 and resid 389 and name CA)	4.14	0.15	0.16
80	assign (segid 3A4 and resid 388 and name N)	(segid 3A4 and resid 389 and name CB)	4.90	0.20	0.20
	assign (segid 3A4 and resid 388 and name N)	(segid 3A4 and resid 389 and name N)	2.72	0.15	0.15
	assign (segid 3A4 and resid 388 and name N)	(segid 3A4 and resid 389 and name O)	5.94	0.20	0.20

	assign (segid 3A4 and resid 388 and name N)	(segid 3A4 and resid 390 and name C)	6.63	0.19	0.18
	assign (segid 3A4 and resid 388 and name N)	(segid 3A4 and resid 390 and name CA)	5.45	0.17	0.18
	assign (segid 3A4 and resid 388 and name N)	(segid 3A4 and resid 390 and name CB)	5.35	0.15	0.14
	assign (segid 3A4 and resid 388 and name N)	(segid 3A4 and resid 390 and name N)	4.34	0.16	0.17
	assign (segid 3A4 and resid 388 and name N)	(segid 3A4 and resid 390 and name O)	6.68	0.26	0.26
5	assign (segid 3A4 and resid 388 and name N)	(segid 3A4 and resid 390 and name O1D)	7.51	0.23	0.23
	assign (segid 3A4 and resid 388 and name O)	(segid 3A4 and resid 388 and name CB)	3.12	0.05	0.05
	assign (segid 3A4 and resid 388 and name O)	(segid 3A4 and resid 389 and name C)	3.59	0.11	0.12
	assign (segid 3A4 and resid 388 and name O)	(segid 3A4 and resid 389 and name CA)	2.78	0.04	0.05
	assign (segid 3A4 and resid 388 and name O)	(segid 3A4 and resid 389 and name CB)	4.07	0.07	0.06
10	assign (segid 3A4 and resid 388 and name O)	(segid 3A4 and resid 389 and name N)	2.25	0.01	0.01
	assign (segid 3A4 and resid 388 and name O)	(segid 3A4 and resid 389 and name O)	4.64	0.14	0.14
	assign (segid 3A4 and resid 388 and name O)	(segid 3A4 and resid 390 and name C)	5.31	0.17	0.18
	assign (segid 3A4 and resid 388 and name O)	(segid 3A4 and resid 390 and name CA)	4.92	0.16	0.15
	assign (segid 3A4 and resid 388 and name O)	(segid 3A4 and resid 390 and name CB)	5.27	0.18	0.19
15	assign (segid 3A4 and resid 388 and name O)	(segid 3A4 and resid 390 and name N)	3.63	0.13	0.13
	assign (segid 3A4 and resid 388 and name O)	(segid 3A4 and resid 390 and name O)	4.74	0.21	0.22
	assign (segid 3A4 and resid 388 and name O)	(segid 3A4 and resid 391 and name C)	7.39	0.23	0.22
	assign (segid 3A4 and resid 388 and name O)	(segid 3A4 and resid 391 and name CA)	7.41	0.19	0.19
	assign (segid 3A4 and resid 388 and name O)	(segid 3A4 and resid 391 and name N)	6.60	0.19	0.18
20	assign (segid 3A4 and resid 388 and name O)	(segid 3A4 and resid 391 and name CBD)	5.81	0.37	0.36
	assign (segid 3A4 and resid 388 and name O)	(segid HEM and resid 1 and name CGD)	4.98	0.37	0.38
	assign (segid 3A4 and resid 388 and name O)	(segid HEM and resid 1 and name O1D)	4.45	0.37	0.37
	assign (segid 3A4 and resid 388 and name O)	(segid HEM and resid 1 and name O2D)	5.22	0.76	0.75
	assign (segid 3A4 and resid 388 and name O)	(segid 3A4 and resid 389 and name CB)	2.51	0.00	0.01
25	assign (segid 3A4 and resid 389 and name C)	(segid 3A4 and resid 389 and name O)	1.24	0.01	0.01
	assign (segid 3A4 and resid 389 and name C)	(segid 3A4 and resid 390 and name C)	2.93	0.07	0.06
	assign (segid 3A4 and resid 389 and name C)	(segid 3A4 and resid 390 and name CA)	2.44	0.03	0.02
	assign (segid 3A4 and resid 389 and name C)	(segid 3A4 and resid 390 and name CB)	3.69	0.04	0.03
	assign (segid 3A4 and resid 389 and name C)	(segid 3A4 and resid 390 and name N)	1.32	0.01	0.02
30	assign (segid 3A4 and resid 389 and name C)	(segid 3A4 and resid 390 and name O)	3.04	0.10	0.11
	assign (segid 3A4 and resid 389 and name C)	(segid 3A4 and resid 391 and name C)	5.58	0.12	0.12
	assign (segid 3A4 and resid 389 and name C)	(segid 3A4 and resid 391 and name CA)	4.93	0.17	0.18
	assign (segid 3A4 and resid 389 and name C)	(segid 3A4 and resid 391 and name CB)	6.17	0.19	0.19
	assign (segid 3A4 and resid 389 and name C)	(segid 3A4 and resid 391 and name N)	3.94	0.18	0.18
35	assign (segid 3A4 and resid 389 and name C)	(segid 3A4 and resid 391 and name O)	6.14	0.24	0.24
	assign (segid 3A4 and resid 389 and name C)	(segid 3A4 and resid 392 and name CA)	6.91	0.17	0.17
	assign (segid 3A4 and resid 389 and name C)	(segid 3A4 and resid 392 and name CB)	7.22	0.16	0.16
	assign (segid 3A4 and resid 389 and name C)	(segid 3A4 and resid 392 and name N)	5.90	0.20	0.19
	assign (segid 3A4 and resid 389 and name C)	(segid HEM and resid 1 and name C1A)	5.79	0.29	0.30
40	assign (segid 3A4 and resid 389 and name C)	(segid HEM and resid 1 and name C2A)	5.67	0.30	0.29
	assign (segid 3A4 and resid 389 and name C)	(segid HEM and resid 1 and name C2D)	7.30	0.25	0.26
	assign (segid 3A4 and resid 389 and name C)	(segid HEM and resid 1 and name C3A)	6.71	0.24	0.25
	assign (segid 3A4 and resid 389 and name C)	(segid HEM and resid 1 and name C3D)	6.15	0.26	0.26
	assign (segid 3A4 and resid 389 and name C)	(segid HEM and resid 1 and name C4A)	7.37	0.20	0.20
45	assign (segid 3A4 and resid 389 and name C)	(segid HEM and resid 1 and name C4D)	6.05	0.27	0.26
	assign (segid 3A4 and resid 389 and name C)	(segid HEM and resid 1 and name CAA)	4.94	0.38	0.38
	assign (segid 3A4 and resid 389 and name C)	(segid HEM and resid 1 and name CAD)	5.47	0.27	0.27
	assign (segid 3A4 and resid 389 and name C)	(segid HEM and resid 1 and name CBA)	4.89	0.66	0.66
	assign (segid 3A4 and resid 389 and name C)	(segid HEM and resid 1 and name CBD)	4.47	0.19	0.20
50	assign (segid 3A4 and resid 389 and name C)	(segid HEM and resid 1 and name CGA)	4.64	0.69	0.68
	assign (segid 3A4 and resid 389 and name C)	(segid HEM and resid 1 and name CGD)	4.25	0.17	0.17
	assign (segid 3A4 and resid 389 and name C)	(segid HEM and resid 1 and name CHA)	5.34	0.35	0.35
	assign (segid 3A4 and resid 389 and name C)	(segid HEM and resid 1 and name CMA)	7.41	0.20	0.20
	assign (segid 3A4 and resid 389 and name C)	(segid HEM and resid 1 and name NA)	6.89	0.24	0.23
55	assign (segid 3A4 and resid 389 and name C)	(segid HEM and resid 1 and name ND)	7.15	0.23	0.23
	assign (segid 3A4 and resid 389 and name C)	(segid HEM and resid 1 and name O1A)	4.48	0.35	0.35
	assign (segid 3A4 and resid 389 and name C)	(segid HEM and resid 1 and name O1D)	4.40	0.28	0.29
	assign (segid 3A4 and resid 389 and name C)	(segid HEM and resid 1 and name O2A)	5.07	1.07	1.07
	assign (segid 3A4 and resid 389 and name C)	(segid HEM and resid 1 and name O2D)	4.44	0.34	0.34
60	assign (segid 3A4 and resid 389 and name C)	(segid 3A4 and resid 389 and name C)	1.53	0.00	0.01
	assign (segid 3A4 and resid 389 and name CA)	(segid 3A4 and resid 389 and name CB)	1.53	0.02	0.01
	assign (segid 3A4 and resid 389 and name CA)	(segid 3A4 and resid 389 and name O)	2.40	0.01	0.01
	assign (segid 3A4 and resid 389 and name CA)	(segid 3A4 and resid 390 and name C)	4.35	0.05	0.05
	assign (segid 3A4 and resid 389 and name CA)	(segid 3A4 and resid 390 and name CA)	3.83	0.04	0.04
65	assign (segid 3A4 and resid 389 and name CA)	(segid 3A4 and resid 390 and name CB)	4.86	0.06	0.05
	assign (segid 3A4 and resid 389 and name CA)	(segid 3A4 and resid 390 and name N)	2.46	0.04	0.05
	assign (segid 3A4 and resid 389 and name CA)	(segid 3A4 and resid 390 and name O)	4.21	0.13	0.12
	assign (segid 3A4 and resid 389 and name CA)	(segid 3A4 and resid 391 and name C)	6.83	0.10	0.10
	assign (segid 3A4 and resid 389 and name CA)	(segid 3A4 and resid 391 and name CA)	6.32	0.15	0.14
70	assign (segid 3A4 and resid 389 and name CA)	(segid 3A4 and resid 391 and name CB)	7.61	0.17	0.18
	assign (segid 3A4 and resid 389 and name CA)	(segid 3A4 and resid 391 and name N)	5.42	0.16	0.15
	assign (segid 3A4 and resid 389 and name CA)	(segid 3A4 and resid 391 and name O)	7.41	0.29	0.29
	assign (segid 3A4 and resid 389 and name CA)	(segid 3A4 and resid 392 and name CA)	7.83	0.16	0.16
	assign (segid 3A4 and resid 389 and name CA)	(segid 3A4 and resid 392 and name CB)	7.90	0.15	0.16
75	assign (segid 3A4 and resid 389 and name CA)	(segid 3A4 and resid 392 and name N)	6.97	0.17	0.17
	assign (segid 3A4 and resid 389 and name CA)	(segid 3A4 and resid 393 and name CA)	11.05	0.14	0.15
	assign (segid 3A4 and resid 389 and name CA)	(segid 3A4 and resid 394 and name CA)	11.47	0.17	0.17
	assign (segid 3A4 and resid 389 and name CA)	(segid 3A4 and resid 394 and name CB)	10.73	0.22	0.21
	assign (segid 3A4 and resid 389 and name CA)	(segid 3A4 and resid 395 and name CA)	11.42	0.25	0.25
80	assign (segid 3A4 and resid 389 and name CA)	(segid 3A4 and resid 396 and name CA)	16.03	0.23	0.22
	assign (segid 3A4 and resid 389 and name CA)	(segid 3A4 and resid 396 and name CB)	15.71	0.36	0.36
	assign (segid 3A4 and resid 389 and name CA)	(segid 3A4 and resid 397 and name CA)	15.77	0.17	0.18

assign (segid 3A4 and resid 389 and name CA) (segid 3A4 and resid 397 and name CB) 14.62 0.20 0.20
 assign (segid 3A4 and resid 389 and name CA) (segid 3A4 and resid 398 and name CA) 17.42 0.20 0.19
 assign (segid 3A4 and resid 389 and name CA) (segid 3A4 and resid 398 and name CB) 16.98 0.21 0.20
 assign (segid 3A4 and resid 389 and name CA) (segid HEM and resid 1 and name C1A) 6.92 0.35 0.36
 assign (segid 3A4 and resid 389 and name CA) (segid HEM and resid 1 and name C2A) 6.78 0.38 0.38
 5 assign (segid 3A4 and resid 389 and name CA) (segid HEM and resid 1 and name C3D) 6.79 0.30 0.31
 assign (segid 3A4 and resid 389 and name CA) (segid HEM and resid 1 and name C4D) 6.94 0.31 0.30
 assign (segid 3A4 and resid 389 and name CA) (segid HEM and resid 1 and name CAA) 5.86 0.48 0.48
 assign (segid 3A4 and resid 389 and name CA) (segid HEM and resid 1 and name CAD) 5.81 0.33 0.33
 assign (segid 3A4 and resid 389 and name CA) (segid HEM and resid 1 and name CBA) 5.69 0.62 0.61
 10 assign (segid 3A4 and resid 389 and name CA) (segid HEM and resid 1 and name CBD) 4.75 0.24 0.23
 assign (segid 3A4 and resid 389 and name CA) (segid HEM and resid 1 and name CGA) 5.12 0.61 0.61
 assign (segid 3A4 and resid 389 and name CA) (segid HEM and resid 1 and name CGD) 4.02 0.23 0.22
 assign (segid 3A4 and resid 389 and name CA) (segid HEM and resid 1 and name CHA) 6.30 0.40 0.40
 assign (segid 3A4 and resid 389 and name CA) (segid HEM and resid 1 and name O1A) 4.84 0.38 0.38
 15 assign (segid 3A4 and resid 389 and name CA) (segid HEM and resid 1 and name O1D) 3.97 0.27 0.27
 assign (segid 3A4 and resid 389 and name CA) (segid HEM and resid 1 and name O2A) 5.39 0.90 0.90
 assign (segid 3A4 and resid 389 and name CA) (segid HEM and resid 1 and name O2D) 4.02 0.41 0.40
 assign (segid 3A4 and resid 389 and name CB) (segid 3A4 and resid 390 and name C) 5.38 0.07 0.06
 assign (segid 3A4 and resid 389 and name CB) (segid 3A4 and resid 390 and name CA) 4.85 0.04 0.04
 20 assign (segid 3A4 and resid 389 and name CB) (segid 3A4 and resid 390 and name CB) 6.00 0.03 0.04
 assign (segid 3A4 and resid 389 and name CB) (segid 3A4 and resid 390 and name N) 3.63 0.04 0.05
 assign (segid 3A4 and resid 389 and name CB) (segid 3A4 and resid 390 and name O) 5.38 0.12 0.11
 assign (segid 3A4 and resid 389 and name CB) (segid 3A4 and resid 391 and name CA) 7.09 0.25 0.26
 assign (segid 3A4 and resid 389 and name CB) (segid 3A4 and resid 391 and name CB) 8.26 0.30 0.31
 25 assign (segid 3A4 and resid 389 and name CB) (segid 3A4 and resid 391 and name N) 6.25 0.24 0.24
 assign (segid 3A4 and resid 389 and name CB) (segid 3A4 and resid 392 and name CA) 8.89 0.19 0.20
 assign (segid 3A4 and resid 389 and name CB) (segid 3A4 and resid 392 and name CB) 8.88 0.20 0.21
 assign (segid 3A4 and resid 389 and name CB) (segid 3A4 and resid 393 and name CA) 11.91 0.26 0.26
 30 assign (segid 3A4 and resid 389 and name CB) (segid 3A4 and resid 394 and name CA) 12.40 0.18 0.19
 assign (segid 3A4 and resid 389 and name CB) (segid 3A4 and resid 394 and name CB) 11.72 0.20 0.21
 assign (segid 3A4 and resid 389 and name CB) (segid 3A4 and resid 395 and name CA) 15.53 0.22 0.22
 assign (segid 3A4 and resid 389 and name CB) (segid 3A4 and resid 396 and name CA) 16.97 0.27 0.27
 assign (segid 3A4 and resid 389 and name CB) (segid 3A4 and resid 396 and name CB) 16.61 0.42 0.41
 35 assign (segid 3A4 and resid 389 and name CB) (segid 3A4 and resid 397 and name CA) 16.48 0.28 0.29
 assign (segid 3A4 and resid 389 and name CB) (segid 3A4 and resid 397 and name CB) 15.27 0.31 0.31
 assign (segid 3A4 and resid 389 and name CB) (segid 3A4 and resid 398 and name CA) 18.26 0.23 0.23
 assign (segid 3A4 and resid 389 and name CB) (segid 3A4 and resid 398 and name CB) 17.89 0.21 0.20
 assign (segid 3A4 and resid 389 and name CB) (segid HEM and resid 1 and name C1A) 6.88 0.50 0.51
 40 assign (segid 3A4 and resid 389 and name CB) (segid HEM and resid 1 and name C2A) 6.57 0.53 0.52
 assign (segid 3A4 and resid 389 and name CB) (segid HEM and resid 1 and name C3D) 6.96 0.44 0.44
 assign (segid 3A4 and resid 389 and name CB) (segid HEM and resid 1 and name C4D) 7.08 0.46 0.46
 assign (segid 3A4 and resid 389 and name CB) (segid HEM and resid 1 and name CAA) 5.42 0.60 0.59
 assign (segid 3A4 and resid 389 and name CB) (segid HEM and resid 1 and name CAD) 5.87 0.43 0.43
 45 assign (segid 3A4 and resid 389 and name CB) (segid HEM and resid 1 and name CBA) 5.13 0.65 0.65
 assign (segid 3A4 and resid 389 and name CB) (segid HEM and resid 1 and name CBD) 5.12 0.33 0.33
 assign (segid 3A4 and resid 389 and name CB) (segid HEM and resid 1 and name CGA) 4.32 0.59 0.60
 assign (segid 3A4 and resid 389 and name CB) (segid HEM and resid 1 and name CGD) 4.27 0.30 0.29
 assign (segid 3A4 and resid 389 and name CB) (segid HEM and resid 1 and name CHA) 6.30 0.54 0.53
 50 assign (segid 3A4 and resid 389 and name CB) (segid HEM and resid 1 and name O1A) 3.98 0.45 0.46
 assign (segid 3A4 and resid 389 and name CB) (segid HEM and resid 1 and name O1D) 4.37 0.41 0.41
 assign (segid 3A4 and resid 389 and name CB) (segid HEM and resid 1 and name O2A) 4.52 0.77 0.76
 assign (segid 3A4 and resid 389 and name CB) (segid HEM and resid 1 and name O2D) 3.97 0.33 0.34
 assign (segid 3A4 and resid 389 and name N) (segid 3A4 and resid 389 and name C) 2.48 0.04 0.04
 55 assign (segid 3A4 and resid 389 and name N) (segid 3A4 and resid 389 and name CA) 1.45 0.01 0.02
 assign (segid 3A4 and resid 389 and name N) (segid 3A4 and resid 389 and name CB) 2.44 0.03 0.02
 assign (segid 3A4 and resid 389 and name N) (segid 3A4 and resid 389 and name O) 3.60 0.04 0.04
 assign (segid 3A4 and resid 389 and name N) (segid 3A4 and resid 390 and name C) 5.02 0.08 0.07
 assign (segid 3A4 and resid 389 and name N) (segid 3A4 and resid 390 and name CA) 4.19 0.08 0.08
 60 assign (segid 3A4 and resid 389 and name N) (segid 3A4 and resid 390 and name CB) 4.81 0.08 0.08
 assign (segid 3A4 and resid 389 and name N) (segid 3A4 and resid 390 and name N) 2.75 0.08 0.08
 assign (segid 3A4 and resid 389 and name N) (segid 3A4 and resid 390 and name O) 4.92 0.16 0.17
 assign (segid 3A4 and resid 389 and name N) (segid 3A4 and resid 391 and name C) 7.64 0.14 0.15
 assign (segid 3A4 and resid 389 and name N) (segid 3A4 and resid 391 and name CA) 7.24 0.08 0.07
 65 assign (segid 3A4 and resid 389 and name N) (segid 3A4 and resid 391 and name N) 6.19 0.09 0.08
 assign (segid 3A4 and resid 389 and name N) (segid HEM and resid 1 and name CAA) 6.99 0.50 0.49
 assign (segid 3A4 and resid 389 and name N) (segid HEM and resid 1 and name CAD) 7.19 0.31 0.32
 assign (segid 3A4 and resid 389 and name N) (segid HEM and resid 1 and name CBD) 6.04 0.22 0.22
 assign (segid 3A4 and resid 389 and name N) (segid HEM and resid 1 and name CGA) 6.05 0.74 0.74
 70 assign (segid 3A4 and resid 389 and name N) (segid HEM and resid 1 and name CGD) 5.25 0.24 0.24
 assign (segid 3A4 and resid 389 and name N) (segid HEM and resid 1 and name O1A) 5.66 0.52 0.52
 assign (segid 3A4 and resid 389 and name N) (segid HEM and resid 1 and name O1D) 5.02 0.23 0.23
 assign (segid 3A4 and resid 389 and name N) (segid HEM and resid 1 and name O2D) 5.25 0.50 0.50
 assign (segid 3A4 and resid 389 and name N) (segid 3A4 and resid 389 and name CB) 2.85 0.03 0.03
 75 assign (segid 3A4 and resid 389 and name O) (segid 3A4 and resid 390 and name C) 2.80 0.12 0.13
 assign (segid 3A4 and resid 389 and name O) (segid 3A4 and resid 390 and name CA) 2.75 0.03 0.04
 assign (segid 3A4 and resid 389 and name O) (segid 3A4 and resid 390 and name CB) 4.22 0.04 0.05
 assign (segid 3A4 and resid 389 and name O) (segid 3A4 and resid 390 and name N) 2.23 0.03 0.03
 assign (segid 3A4 and resid 389 and name O) (segid 3A4 and resid 390 and name O) 3.03 0.11 0.11
 80 assign (segid 3A4 and resid 389 and name O) (segid 3A4 and resid 391 and name C) 5.15 0.30 0.30
 assign (segid 3A4 and resid 389 and name O) (segid 3A4 and resid 391 and name CA) 4.30 0.33 0.33
 assign (segid 3A4 and resid 389 and name O) (segid 3A4 and resid 391 and name CB) 5.46 0.32 0.32
 assign (segid 3A4 and resid 389 and name O) (segid 3A4 and resid 391 and name N) 3.49 0.29 0.30

	assign (segid 3A4 and resid 38 and name CA) (segid 3A4 and resid 339 and name CA)	17.78	0.47	0.47
	assign (segid 3A4 and resid 38 and name CA) (segid 3A4 and resid 340 and name CA)	18.37	0.44	0.45
	assign (segid 3A4 and resid 38 and name CA) (segid 3A4 and resid 341 and name CA)	15.85	0.42	0.42
	assign (segid 3A4 and resid 38 and name CA) (segid 3A4 and resid 341 and name CB)	14.97	0.44	0.45
5	assign (segid 3A4 and resid 38 and name CA) (segid 3A4 and resid 342 and name CA)	14.69	0.41	0.40
	assign (segid 3A4 and resid 38 and name CA) (segid 3A4 and resid 343 and name CA)	11.19	0.33	0.34
	assign (segid 3A4 and resid 38 and name CA) (segid 3A4 and resid 343 and name CB)	10.12	0.43	0.44
	assign (segid 3A4 and resid 38 and name CA) (segid 3A4 and resid 344 and name CA)	11.14	0.21	0.21
	assign (segid 3A4 and resid 38 and name CA) (segid 3A4 and resid 344 and name CB)	12.15	0.24	0.24
10	assign (segid 3A4 and resid 38 and name CA) (segid 3A4 and resid 345 and name CA)	8.63	0.48	0.48
	assign (segid 3A4 and resid 38 and name CA) (segid 3A4 and resid 345 and name CB)	8.31	0.61	0.61
	assign (segid 3A4 and resid 38 and name CA) (segid 3A4 and resid 346 and name CA)	10.13	0.52	0.53
	assign (segid 3A4 and resid 38 and name CA) (segid 3A4 and resid 346 and name CB)	10.33	0.50	0.50
	assign (segid 3A4 and resid 38 and name CA) (segid 3A4 and resid 347 and name CA)	10.85	0.60	0.60
15	assign (segid 3A4 and resid 38 and name CA) (segid 3A4 and resid 347 and name CB)	11.88	0.66	0.65
	assign (segid 3A4 and resid 38 and name CA) (segid 3A4 and resid 348 and name CA)	13.26	0.55	0.54
	assign (segid 3A4 and resid 38 and name CA) (segid 3A4 and resid 349 and name CA)	11.01	0.46	0.46
	assign (segid 3A4 and resid 38 and name CA) (segid 3A4 and resid 349 and name CB)	10.29	0.55	0.56
	assign (segid 3A4 and resid 38 and name CA) (segid 3A4 and resid 350 and name CA)	9.02	0.49	0.49
20	assign (segid 3A4 and resid 38 and name CA) (segid 3A4 and resid 350 and name CB)	8.47	0.62	0.62
	assign (segid 3A4 and resid 38 and name CA) (segid 3A4 and resid 351 and name CA)	12.52	0.55	0.54
	assign (segid 3A4 and resid 38 and name CA) (segid 3A4 and resid 352 and name CA)	13.67	0.47	0.47
	assign (segid 3A4 and resid 38 and name CA) (segid 3A4 and resid 352 and name CB)	14.30	0.43	0.44
	assign (segid 3A4 and resid 38 and name CA) (segid 3A4 and resid 353 and name CA)	11.34	0.57	0.57
25	assign (segid 3A4 and resid 38 and name CA) (segid 3A4 and resid 353 and name CB)	10.00	0.70	0.70
	assign (segid 3A4 and resid 38 and name CA) (segid 3A4 and resid 354 and name CA)	14.15	0.65	0.64
	assign (segid 3A4 and resid 38 and name CA) (segid 3A4 and resid 354 and name CB)	14.87	0.61	0.62
	assign (segid 3A4 and resid 38 and name CA) (segid 3A4 and resid 355 and name CA)	12.68	1.10	1.10
	assign (segid 3A4 and resid 38 and name CA) (segid 3A4 and resid 355 and name CB)	11.54	1.20	1.20
30	assign (segid 3A4 and resid 38 and name CA) (segid 3A4 and resid 356 and name CA)	12.66	0.97	0.97
	assign (segid 3A4 and resid 38 and name CA) (segid 3A4 and resid 356 and name CB)	11.58	0.93	0.94
	assign (segid 3A4 and resid 38 and name CA) (segid 3A4 and resid 357 and name CA)	15.63	0.84	0.84
	assign (segid 3A4 and resid 38 and name CA) (segid 3A4 and resid 357 and name CB)	15.60	0.80	0.80
	assign (segid 3A4 and resid 38 and name CA) (segid 3A4 and resid 360 and name CA)	17.88	0.62	0.62
35	assign (segid 3A4 and resid 38 and name CA) (segid 3A4 and resid 360 and name CB)	16.52	0.64	0.64
	assign (segid 3A4 and resid 38 and name CA) (segid 3A4 and resid 381 and name CA)	13.49	0.57	0.56
	assign (segid 3A4 and resid 38 and name CA) (segid 3A4 and resid 382 and name CA)	12.17	0.68	0.68
	assign (segid 3A4 and resid 38 and name CA) (segid 3A4 and resid 382 and name CB)	10.73	0.68	0.68
	assign (segid 3A4 and resid 38 and name CA) (segid 3A4 and resid 383 and name CA)	15.24	0.60	0.60
40	assign (segid 3A4 and resid 38 and name CA) (segid 3A4 and resid 384 and name CA)	16.41	0.67	0.67
	assign (segid 3A4 and resid 38 and name CA) (segid 3A4 and resid 384 and name CB)	17.37	0.67	0.66
	assign (segid 3A4 and resid 38 and name CA) (segid 3A4 and resid 385 and name CA)	13.27	0.80	0.81
	assign (segid 3A4 and resid 38 and name CA) (segid 3A4 and resid 386 and name CA)	12.04	0.84	0.85
45	assign (segid 3A4 and resid 38 and name CA) (segid 3A4 and resid 387 and name CA)	13.22	1.13	1.13
	assign (segid 3A4 and resid 38 and name CA) (segid 3A4 and resid 388 and name CA)	16.46	1.16	1.16
	assign (segid 3A4 and resid 38 and name CA) (segid 3A4 and resid 388 and name CB)	16.88	1.26	1.26
	assign (segid 3A4 and resid 38 and name CA) (segid 3A4 and resid 389 and name CA)	16.69	0.84	0.84
	assign (segid 3A4 and resid 38 and name CA) (segid 3A4 and resid 389 and name CB)	16.15	0.76	0.77
50	assign (segid 3A4 and resid 38 and name CA) (segid 3A4 and resid 38 and name C)	1.52	0.00	0.01
	assign (segid 3A4 and resid 38 and name CA) (segid 3A4 and resid 38 and name CB)	1.51	0.01	0.01
	assign (segid 3A4 and resid 38 and name CA) (segid 3A4 and resid 38 and name O)	2.40	0.01	0.01
	assign (segid 3A4 and resid 38 and name CA) (segid 3A4 and resid 390 and name CA)	16.44	0.84	0.83
	assign (segid 3A4 and resid 38 and name CA) (segid 3A4 and resid 390 and name CB)	16.38	0.87	0.87
	assign (segid 3A4 and resid 38 and name CA) (segid 3A4 and resid 39 and name C)	4.40	0.07	0.06
55	assign (segid 3A4 and resid 38 and name CA) (segid 3A4 and resid 39 and name CA)	3.81	0.01	0.01
	assign (segid 3A4 and resid 38 and name CA) (segid 3A4 and resid 39 and name CB)	4.87	0.02	0.02
	assign (segid 3A4 and resid 38 and name CA) (segid 3A4 and resid 39 and name N)	2.44	0.02	0.01
	assign (segid 3A4 and resid 38 and name CA) (segid 3A4 and resid 39 and name O)	5.25	0.08	0.08
	assign (segid 3A4 and resid 38 and name CA) (segid 3A4 and resid 40 and name C)	5.53	0.13	0.12
60	assign (segid 3A4 and resid 38 and name CA) (segid 3A4 and resid 40 and name CA)	5.53	0.14	0.14
	assign (segid 3A4 and resid 38 and name CA) (segid 3A4 and resid 40 and name CB)	5.98	0.16	0.17
	assign (segid 3A4 and resid 38 and name CA) (segid 3A4 and resid 40 and name N)	4.46	0.11	0.12
	assign (segid 3A4 and resid 38 and name CA) (segid 3A4 and resid 40 and name O)	6.62	0.10	0.10
	assign (segid 3A4 and resid 38 and name CA) (segid 3A4 and resid 41 and name C)	5.66	0.09	0.08
65	assign (segid 3A4 and resid 38 and name CA) (segid 3A4 and resid 41 and name CA)	5.06	0.12	0.13
	assign (segid 3A4 and resid 38 and name CA) (segid 3A4 and resid 41 and name CB)	4.36	0.12	0.11
	assign (segid 3A4 and resid 38 and name CA) (segid 3A4 and resid 41 and name N)	4.56	0.16	0.16
	assign (segid 3A4 and resid 38 and name CA) (segid 3A4 and resid 41 and name O)	6.84	0.08	0.08
	assign (segid 3A4 and resid 38 and name CA) (segid 3A4 and resid 42 and name C)	7.32	0.07	0.06
70	assign (segid 3A4 and resid 38 and name CA) (segid 3A4 and resid 42 and name CA)	6.14	0.05	0.06
	assign (segid 3A4 and resid 38 and name CA) (segid 3A4 and resid 42 and name CB)	5.80	0.09	0.10
	assign (segid 3A4 and resid 38 and name CA) (segid 3A4 and resid 42 and name N)	5.14	0.06	0.06
	assign (segid 3A4 and resid 38 and name CB) (segid 3A4 and resid 314 and name CA)	17.85	0.43	0.42
	assign (segid 3A4 and resid 38 and name CB) (segid 3A4 and resid 314 and name CB)	17.95	0.43	0.43
75	assign (segid 3A4 and resid 38 and name CB) (segid 3A4 and resid 317 and name CA)	17.70	0.50	0.50
	assign (segid 3A4 and resid 38 and name CB) (segid 3A4 and resid 319 and name CA)	17.62	0.81	0.82
	assign (segid 3A4 and resid 38 and name CB) (segid 3A4 and resid 319 and name CB)	17.61	0.94	0.93
	assign (segid 3A4 and resid 38 and name CB) (segid 3A4 and resid 322 and name CA)	13.50	0.89	0.89
	assign (segid 3A4 and resid 38 and name CB) (segid 3A4 and resid 323 and name CA)	13.09	0.50	0.50
80	assign (segid 3A4 and resid 38 and name CB) (segid 3A4 and resid 323 and name CB)	11.90	0.49	0.49
	assign (segid 3A4 and resid 38 and name CB) (segid 3A4 and resid 324 and name CA)	14.68	0.42	0.42
	assign (segid 3A4 and resid 38 and name CB) (segid 3A4 and resid 324 and name CB)	16.20	0.39	0.40
	assign (segid 3A4 and resid 38 and name CB) (segid 3A4 and resid 325 and name CA)	14.12	0.44	0.43

	assign (segid 3A4 and resid 38 and name CB) (segid 3A4 and resid 325 and name CB)	13.60	0.38	0.37
	assign (segid 3A4 and resid 38 and name CB) (segid 3A4 and resid 326 and name CA)	17.24	0.50	0.51
	assign (segid 3A4 and resid 38 and name CB) (segid 3A4 and resid 326 and name CB)	17.58	0.57	0.57
	assign (segid 3A4 and resid 38 and name CB) (segid 3A4 and resid 327 and name CA)	17.37	0.71	0.71
	assign (segid 3A4 and resid 38 and name CB) (segid 3A4 and resid 327 and name CB)	17.71	0.74	0.74
5	assign (segid 3A4 and resid 38 and name CB) (segid 3A4 and resid 328 and name CA)	15.97	0.71	0.71
	assign (segid 3A4 and resid 38 and name CB) (segid 3A4 and resid 328 and name CB)	16.93	0.76	0.77
	assign (segid 3A4 and resid 38 and name CB) (segid 3A4 and resid 329 and name CA)	12.79	0.81	0.81
	assign (segid 3A4 and resid 38 and name CB) (segid 3A4 and resid 329 and name CB)	12.05	0.73	0.73
10	assign (segid 3A4 and resid 38 and name CB) (segid 3A4 and resid 330 and name CA)	10.98	1.10	1.10
	assign (segid 3A4 and resid 38 and name CB) (segid 3A4 and resid 330 and name CB)	11.94	1.18	1.19
	assign (segid 3A4 and resid 38 and name CB) (segid 3A4 and resid 331 and name CA)	7.25	1.10	1.09
	assign (segid 3A4 and resid 38 and name CB) (segid 3A4 and resid 331 and name CB)	6.50	1.06	1.06
	assign (segid 3A4 and resid 38 and name CB) (segid 3A4 and resid 332 and name CA)	7.00	1.13	1.13
15	assign (segid 3A4 and resid 38 and name CB) (segid 3A4 and resid 333 and name CA)	10.43	0.90	0.90
	assign (segid 3A4 and resid 38 and name CB) (segid 3A4 and resid 335 and name CA)	10.31	0.88	0.88
	assign (segid 3A4 and resid 38 and name CB) (segid 3A4 and resid 336 and name CA)	12.49	0.73	0.73
	assign (segid 3A4 and resid 38 and name CB) (segid 3A4 and resid 336 and name CB)	13.91	0.74	0.75
	assign (segid 3A4 and resid 38 and name CB) (segid 3A4 and resid 337 and name CA)	12.29	0.65	0.66
20	assign (segid 3A4 and resid 38 and name CB) (segid 3A4 and resid 337 and name CB)	11.19	0.61	0.60
	assign (segid 3A4 and resid 38 and name CB) (segid 3A4 and resid 338 and name CA)	15.87	0.60	0.61
	assign (segid 3A4 and resid 38 and name CB) (segid 3A4 and resid 338 and name CB)	16.90	0.61	0.61
	assign (segid 3A4 and resid 38 and name CB) (segid 3A4 and resid 339 and name CA)	17.43	0.53	0.52
	assign (segid 3A4 and resid 38 and name CB) (segid 3A4 and resid 340 and name CA)	17.96	0.47	0.47
25	assign (segid 3A4 and resid 38 and name CB) (segid 3A4 and resid 341 and name CA)	15.22	0.46	0.46
	assign (segid 3A4 and resid 38 and name CB) (segid 3A4 and resid 341 and name CB)	14.28	0.47	0.48
	assign (segid 3A4 and resid 38 and name CB) (segid 3A4 and resid 342 and name CA)	14.09	0.46	0.45
	assign (segid 3A4 and resid 38 and name CB) (segid 3A4 and resid 343 and name CA)	10.59	0.40	0.41
	assign (segid 3A4 and resid 38 and name CB) (segid 3A4 and resid 343 and name CB)	9.62	0.51	0.52
30	assign (segid 3A4 and resid 38 and name CB) (segid 3A4 and resid 344 and name CA)	10.56	0.20	0.20
	assign (segid 3A4 and resid 38 and name CB) (segid 3A4 and resid 344 and name CB)	11.45	0.22	0.23
	assign (segid 3A4 and resid 38 and name CB) (segid 3A4 and resid 345 and name CA)	8.35	0.40	0.40
	assign (segid 3A4 and resid 38 and name CB) (segid 3A4 and resid 345 and name CB)	8.28	0.54	0.54
35	assign (segid 3A4 and resid 38 and name CB) (segid 3A4 and resid 346 and name CA)	9.75	0.51	0.51
	assign (segid 3A4 and resid 38 and name CB) (segid 3A4 and resid 346 and name CB)	9.77	0.54	0.53
	assign (segid 3A4 and resid 38 and name CB) (segid 3A4 and resid 347 and name CA)	10.96	0.51	0.50
	assign (segid 3A4 and resid 38 and name CB) (segid 3A4 and resid 347 and name CB)	12.08	0.55	0.55
	assign (segid 3A4 and resid 38 and name CB) (segid 3A4 and resid 348 and name CA)	13.13	0.48	0.48
40	assign (segid 3A4 and resid 38 and name CB) (segid 3A4 and resid 349 and name CA)	10.65	0.43	0.43
	assign (segid 3A4 and resid 38 and name CB) (segid 3A4 and resid 349 and name CB)	9.77	0.54	0.53
	assign (segid 3A4 and resid 38 and name CB) (segid 3A4 and resid 350 and name CA)	9.13	0.45	0.45
	assign (segid 3A4 and resid 38 and name CB) (segid 3A4 and resid 350 and name CB)	8.76	0.60	0.60
	assign (segid 3A4 and resid 38 and name CB) (segid 3A4 and resid 351 and name CA)	12.76	0.47	0.48
45	assign (segid 3A4 and resid 38 and name CB) (segid 3A4 and resid 352 and name CA)	13.59	0.43	0.42
	assign (segid 3A4 and resid 38 and name CB) (segid 3A4 and resid 352 and name CB)	14.08	0.37	0.38
	assign (segid 3A4 and resid 38 and name CB) (segid 3A4 and resid 353 and name CA)	11.26	0.56	0.57
	assign (segid 3A4 and resid 38 and name CB) (segid 3A4 and resid 353 and name CB)	10.02	0.71	0.71
	assign (segid 3A4 and resid 38 and name CB) (segid 3A4 and resid 354 and name CA)	14.06	0.62	0.63
	assign (segid 3A4 and resid 38 and name CB) (segid 3A4 and resid 354 and name CB)	14.67	0.61	0.60
50	assign (segid 3A4 and resid 38 and name CB) (segid 3A4 and resid 355 and name CA)	12.83	1.09	1.09
	assign (segid 3A4 and resid 38 and name CB) (segid 3A4 and resid 355 and name CB)	11.67	1.21	1.22
	assign (segid 3A4 and resid 38 and name CB) (segid 3A4 and resid 356 and name CA)	13.15	0.93	0.92
	assign (segid 3A4 and resid 38 and name CB) (segid 3A4 and resid 356 and name CB)	12.13	0.89	0.89
	assign (segid 3A4 and resid 38 and name CB) (segid 3A4 and resid 357 and name CA)	15.99	0.79	0.79
55	assign (segid 3A4 and resid 38 and name CB) (segid 3A4 and resid 357 and name CB)	15.94	0.75	0.74
	assign (segid 3A4 and resid 38 and name CB) (segid 3A4 and resid 360 and name CA)	17.88	0.58	0.57
	assign (segid 3A4 and resid 38 and name CB) (segid 3A4 and resid 360 and name CB)	16.46	0.60	0.60
	assign (segid 3A4 and resid 38 and name CB) (segid 3A4 and resid 381 and name CA)	14.28	0.49	0.50
	assign (segid 3A4 and resid 38 and name CB) (segid 3A4 and resid 382 and name CA)	12.95	0.58	0.57
60	assign (segid 3A4 and resid 38 and name CB) (segid 3A4 and resid 382 and name CB)	11.48	0.58	0.59
	assign (segid 3A4 and resid 38 and name CB) (segid 3A4 and resid 383 and name CA)	15.81	0.48	0.47
	assign (segid 3A4 and resid 38 and name CB) (segid 3A4 and resid 384 and name CA)	17.15	0.56	0.56
	assign (segid 3A4 and resid 38 and name CB) (segid 3A4 and resid 384 and name CB)	18.19	0.56	0.56
	assign (segid 3A4 and resid 38 and name CB) (segid 3A4 and resid 385 and name CA)	14.05	0.71	0.70
65	assign (segid 3A4 and resid 38 and name CB) (segid 3A4 and resid 386 and name CA)	13.11	0.71	0.72
	assign (segid 3A4 and resid 38 and name CB) (segid 3A4 and resid 387 and name CA)	14.36	1.07	1.07
	assign (segid 3A4 and resid 38 and name CB) (segid 3A4 and resid 389 and name CA)	17.54	0.75	0.75
	assign (segid 3A4 and resid 38 and name CB) (segid 3A4 and resid 389 and name CB)	16.91	0.69	0.69
	assign (segid 3A4 and resid 38 and name CB) (segid 3A4 and resid 390 and name CA)	17.38	0.74	0.75
70	assign (segid 3A4 and resid 38 and name CB) (segid 3A4 and resid 390 and name CB)	17.41	0.79	0.79
	assign (segid 3A4 and resid 38 and name CB) (segid 3A4 and resid 39 and name C)	5.44	0.05	0.04
	assign (segid 3A4 and resid 38 and name CB) (segid 3A4 and resid 39 and name CA)	4.52	0.04	0.03
	assign (segid 3A4 and resid 38 and name CB) (segid 3A4 and resid 39 and name CB)	5.39	0.08	0.08
	assign (segid 3A4 and resid 38 and name CB) (segid 3A4 and resid 39 and name N)	3.20	0.04	0.05
75	assign (segid 3A4 and resid 38 and name CB) (segid 3A4 and resid 39 and name O)	6.24	0.08	0.07
	assign (segid 3A4 and resid 38 and name CB) (segid 3A4 and resid 40 and name C)	6.91	0.11	0.12
	assign (segid 3A4 and resid 38 and name CB) (segid 3A4 and resid 40 and name CA)	6.90	0.11	0.10
	assign (segid 3A4 and resid 38 and name CB) (segid 3A4 and resid 40 and name CB)	7.42	0.14	0.13
	assign (segid 3A4 and resid 38 and name CB) (segid 3A4 and resid 40 and name N)	5.71	0.08	0.09
80	assign (segid 3A4 and resid 38 and name CB) (segid 3A4 and resid 41 and name C)	6.75	0.13	0.13
	assign (segid 3A4 and resid 38 and name CB) (segid 3A4 and resid 41 and name CA)	6.35	0.16	0.17
	assign (segid 3A4 and resid 38 and name CB) (segid 3A4 and resid 41 and name CB)	5.55	0.18	0.17
	assign (segid 3A4 and resid 38 and name CB) (segid 3A4 and resid 41 and name N)	5.96	0.17	0.18

	assign (segid 3A4 and resid 38 and name CB)	(segid 3A4 and resid 42 and name CA)	6.86	0.07	0.06
	assign (segid 3A4 and resid 38 and name CB)	(segid 3A4 and resid 42 and name CB)	6.24	0.07	0.08
	assign (segid 3A4 and resid 38 and name CB)	(segid 3A4 and resid 42 and name N)	6.08	0.11	0.10
	assign (segid 3A4 and resid 38 and name N)	(segid 3A4 and resid 38 and name C)	2.47	0.03	0.03
	assign (segid 3A4 and resid 38 and name N)	(segid 3A4 and resid 38 and name CA)	1.45	0.00	0.00
5	assign (segid 3A4 and resid 38 and name N)	(segid 3A4 and resid 38 and name CB)	2.43	0.02	0.03
	assign (segid 3A4 and resid 38 and name N)	(segid 3A4 and resid 38 and name O)	3.54	0.05	0.04
	assign (segid 3A4 and resid 38 and name N)	(segid 3A4 and resid 39 and name C)	4.71	0.04	0.03
	assign (segid 3A4 and resid 38 and name N)	(segid 3A4 and resid 39 and name CA)	4.22	0.04	0.03
	assign (segid 3A4 and resid 38 and name N)	(segid 3A4 and resid 39 and name CB)	4.98	0.04	0.03
10	assign (segid 3A4 and resid 38 and name N)	(segid 3A4 and resid 39 and name N)	2.80	0.03	0.04
	assign (segid 3A4 and resid 38 and name N)	(segid 3A4 and resid 39 and name O)	5.75	0.04	0.04
	assign (segid 3A4 and resid 38 and name N)	(segid 3A4 and resid 40 and name C)	5.71	0.13	0.12
	assign (segid 3A4 and resid 38 and name N)	(segid 3A4 and resid 40 and name CA)	5.44	0.12	0.12
	assign (segid 3A4 and resid 38 and name N)	(segid 3A4 and resid 40 and name CB)	5.55	0.14	0.15
15	assign (segid 3A4 and resid 38 and name N)	(segid 3A4 and resid 40 and name N)	4.42	0.09	0.08
	assign (segid 3A4 and resid 38 and name N)	(segid 3A4 and resid 40 and name O)	6.90	0.12	0.11
	assign (segid 3A4 and resid 38 and name N)	(segid 3A4 and resid 41 and name C)	6.45	0.13	0.13
	assign (segid 3A4 and resid 38 and name N)	(segid 3A4 and resid 41 and name CA)	5.60	0.16	0.15
	assign (segid 3A4 and resid 38 and name N)	(segid 3A4 and resid 41 and name CB)	4.97	0.18	0.19
20	assign (segid 3A4 and resid 38 and name N)	(segid 3A4 and resid 41 and name N)	4.86	0.15	0.15
	assign (segid 3A4 and resid 38 and name N)	(segid 3A4 and resid 41 and name O)	7.65	0.13	0.13
	assign (segid 3A4 and resid 38 and name N)	(segid 3A4 and resid 42 and name CA)	7.23	0.11	0.12
	assign (segid 3A4 and resid 38 and name N)	(segid 3A4 and resid 42 and name CB)	7.00	0.11	0.10
	assign (segid 3A4 and resid 38 and name N)	(segid 3A4 and resid 42 and name N)	6.10	0.11	0.11
25	assign (segid 3A4 and resid 38 and name N)	(segid 3A4 and resid 331 and name CB)	6.56	0.80	0.80
	assign (segid 3A4 and resid 38 and name O)	(segid 3A4 and resid 38 and name CB)	3.24	0.06	0.05
	assign (segid 3A4 and resid 38 and name O)	(segid 3A4 and resid 39 and name C)	3.02	0.05	0.06
	assign (segid 3A4 and resid 38 and name O)	(segid 3A4 and resid 39 and name CA)	2.77	0.01	0.01
	assign (segid 3A4 and resid 38 and name O)	(segid 3A4 and resid 39 and name CB)	4.27	0.01	0.02
30	assign (segid 3A4 and resid 38 and name O)	(segid 3A4 and resid 39 and name N)	2.26	0.01	0.00
	assign (segid 3A4 and resid 38 and name O)	(segid 3A4 and resid 39 and name O)	3.40	0.07	0.07
	assign (segid 3A4 and resid 38 and name O)	(segid 3A4 and resid 40 and name C)	4.21	0.10	0.11
	assign (segid 3A4 and resid 38 and name O)	(segid 3A4 and resid 40 and name CA)	4.54	0.12	0.13
	assign (segid 3A4 and resid 38 and name O)	(segid 3A4 and resid 40 and name CB)	5.53	0.13	0.13
35	assign (segid 3A4 and resid 38 and name O)	(segid 3A4 and resid 40 and name N)	3.60	0.11	0.11
	assign (segid 3A4 and resid 38 and name O)	(segid 3A4 and resid 40 and name O)	5.07	0.03	0.03
	assign (segid 3A4 and resid 38 and name O)	(segid 3A4 and resid 41 and name C)	3.81	0.12	0.12
	assign (segid 3A4 and resid 38 and name O)	(segid 3A4 and resid 41 and name CA)	3.76	0.18	0.17
	assign (segid 3A4 and resid 38 and name O)	(segid 3A4 and resid 41 and name CB)	3.55	0.19	0.20
40	assign (segid 3A4 and resid 38 and name O)	(segid 3A4 and resid 41 and name N)	3.39	0.21	0.20
	assign (segid 3A4 and resid 38 and name O)	(segid 3A4 and resid 41 and name O)	4.98	0.10	0.11
	assign (segid 3A4 and resid 38 and name O)	(segid 3A4 and resid 42 and name C)	4.97	0.04	0.04
	assign (segid 3A4 and resid 38 and name O)	(segid 3A4 and resid 42 and name CA)	3.83	0.04	0.04
	assign (segid 3A4 and resid 38 and name O)	(segid 3A4 and resid 42 and name CB)	3.49	0.11	0.11
45	assign (segid 3A4 and resid 38 and name O)	(segid 3A4 and resid 42 and name N)	2.96	0.07	0.08
	assign (segid 3A4 and resid 38 and name O)	(segid 3A4 and resid 42 and name O)	6.09	0.02	0.03
	assign (segid 3A4 and resid 38 and name O)	(segid 3A4 and resid 42 and name CB)	2.52	0.02	0.02
	assign (segid 3A4 and resid 390 and name C)	(segid 3A4 and resid 390 and name O)	1.23	0.01	0.01
	assign (segid 3A4 and resid 390 and name C)	(segid 3A4 and resid 391 and name C)	2.98	0.04	0.03
50	assign (segid 3A4 and resid 390 and name C)	(segid 3A4 and resid 391 and name CA)	2.44	0.01	0.02
	assign (segid 3A4 and resid 390 and name C)	(segid 3A4 and resid 391 and name CB)	3.69	0.01	0.02
	assign (segid 3A4 and resid 390 and name C)	(segid 3A4 and resid 391 and name N)	1.34	0.01	0.00
	assign (segid 3A4 and resid 390 and name C)	(segid 3A4 and resid 391 and name O)	3.38	0.18	0.17
	assign (segid 3A4 and resid 390 and name C)	(segid 3A4 and resid 392 and name C)	5.93	0.13	0.12
55	assign (segid 3A4 and resid 390 and name C)	(segid 3A4 and resid 392 and name CA)	4.83	0.07	0.08
	assign (segid 3A4 and resid 390 and name C)	(segid 3A4 and resid 392 and name CB)	5.68	0.09	0.08
	assign (segid 3A4 and resid 390 and name C)	(segid 3A4 and resid 392 and name N)	3.73	0.11	0.10
	assign (segid 3A4 and resid 390 and name C)	(segid 3A4 and resid 392 and name O)	6.75	0.16	0.16
	assign (segid 3A4 and resid 390 and name C)	(segid 3A4 and resid 393 and name C)	7.59	0.17	0.18
60	assign (segid 3A4 and resid 390 and name C)	(segid 3A4 and resid 393 and name CA)	7.46	0.15	0.14
	assign (segid 3A4 and resid 390 and name C)	(segid 3A4 and resid 393 and name N)	6.20	0.11	0.11
	assign (segid 3A4 and resid 390 and name C)	(segid 3A4 and resid 394 and name CA)	7.21	0.19	0.18
	assign (segid 3A4 and resid 390 and name C)	(segid 3A4 and resid 394 and name CB)	6.43	0.20	0.20
	assign (segid 3A4 and resid 390 and name C)	(segid 3A4 and resid 394 and name N)	6.70	0.17	0.17
65	assign (segid 3A4 and resid 390 and name C)	(segid 3A4 and resid 394 and name C)	4.97	0.19	0.20
	assign (segid 3A4 and resid 390 and name C)	(segid HEM and resid 1 and name C1A)	7.67	0.11	0.12
	assign (segid 3A4 and resid 390 and name C)	(segid HEM and resid 1 and name C1B)	6.59	0.16	0.16
	assign (segid 3A4 and resid 390 and name C)	(segid HEM and resid 1 and name C1D)	5.23	0.19	0.18
	assign (segid 3A4 and resid 390 and name C)	(segid HEM and resid 1 and name C2A)	6.52	0.18	0.18
	assign (segid 3A4 and resid 390 and name C)	(segid HEM and resid 1 and name C2D)	5.94	0.15	0.15
70	assign (segid 3A4 and resid 390 and name C)	(segid HEM and resid 1 and name C3A)	5.67	0.19	0.20
	assign (segid 3A4 and resid 390 and name C)	(segid HEM and resid 1 and name C3D)	6.11	0.15	0.15
	assign (segid 3A4 and resid 390 and name C)	(segid HEM and resid 1 and name C4A)	5.23	0.20	0.19
	assign (segid 3A4 and resid 390 and name C)	(segid HEM and resid 1 and name C4D)	5.28	0.23	0.23
	assign (segid 3A4 and resid 390 and name C)	(segid HEM and resid 1 and name CAA)	5.70	0.22	0.21
75	assign (segid 3A4 and resid 390 and name C)	(segid HEM and resid 1 and name CAD)	5.54	0.76	0.77
	assign (segid 3A4 and resid 390 and name C)	(segid HEM and resid 1 and name CBA)	4.79	0.14	0.15
	assign (segid 3A4 and resid 390 and name C)	(segid HEM and resid 1 and name CBD)	6.00	0.79	0.78
	assign (segid 3A4 and resid 390 and name C)	(segid HEM and resid 1 and name CGA)	5.41	0.09	0.09
	assign (segid 3A4 and resid 390 and name C)	(segid HEM and resid 1 and name CGD)	4.79	0.26	0.26
80	assign (segid 3A4 and resid 390 and name C)	(segid HEM and resid 1 and name CHA)	7.08	0.17	0.17
	assign (segid 3A4 and resid 390 and name C)	(segid HEM and resid 1 and name CHB)	7.60	0.14	0.14
	assign (segid 3A4 and resid 390 and name C)	(segid HEM and resid 1 and name CHD)			

	assign (segid 3A4 and resid 390 and name C) (segid HEM and resid 1 and name CMA)	6.85	0.17	0.16
	assign (segid 3A4 and resid 390 and name C) (segid HEM and resid 1 and name CMD)	7.57	0.17	0.18
	assign (segid 3A4 and resid 390 and name C) (segid HEM and resid 1 and name FE)	6.32	0.16	0.16
	assign (segid 3A4 and resid 390 and name C) (segid HEM and resid 1 and name NA)	5.59	0.14	0.14
5	assign (segid 3A4 and resid 390 and name C) (segid HEM and resid 1 and name NB)	7.50	0.12	0.11
	assign (segid 3A4 and resid 390 and name C) (segid HEM and resid 1 and name NC)	7.65	0.13	0.12
	assign (segid 3A4 and resid 390 and name C) (segid HEM and resid 1 and name ND)	5.87	0.17	0.16
	assign (segid 3A4 and resid 390 and name C) (segid HEM and resid 1 and name O1A)	6.07	0.48	0.47
	assign (segid 3A4 and resid 390 and name C) (segid HEM and resid 1 and name O1D)	5.67	0.25	0.25
	assign (segid 3A4 and resid 390 and name C) (segid HEM and resid 1 and name O2D)	5.97	0.35	0.35
10	assign (segid 3A4 and resid 390 and name C) (segid 3A4 and resid 390 and name C)	1.53	0.01	0.00
	assign (segid 3A4 and resid 390 and name CA) (segid 3A4 and resid 390 and name C)	1.53	0.02	0.01
	assign (segid 3A4 and resid 390 and name CA) (segid 3A4 and resid 390 and name O)	2.40	0.02	0.02
	assign (segid 3A4 and resid 390 and name CA) (segid 3A4 and resid 391 and name C)	4.43	0.05	0.05
	assign (segid 3A4 and resid 390 and name CA) (segid 3A4 and resid 391 and name CB)	3.81	0.01	0.01
15	assign (segid 3A4 and resid 390 and name CA) (segid 3A4 and resid 391 and name CB)	4.83	0.03	0.02
	assign (segid 3A4 and resid 390 and name CA) (segid 3A4 and resid 391 and name N)	2.44	0.02	0.02
	assign (segid 3A4 and resid 390 and name CA) (segid 3A4 and resid 391 and name O)	4.64	0.21	0.21
	assign (segid 3A4 and resid 390 and name CA) (segid 3A4 and resid 392 and name C)	7.37	0.12	0.12
	assign (segid 3A4 and resid 390 and name CA) (segid 3A4 and resid 392 and name CA)	6.27	0.08	0.07
20	assign (segid 3A4 and resid 390 and name CA) (segid 3A4 and resid 392 and name CB)	7.08	0.09	0.09
	assign (segid 3A4 and resid 390 and name CA) (segid 3A4 and resid 392 and name N)	5.23	0.10	0.10
	assign (segid 3A4 and resid 390 and name CA) (segid 3A4 and resid 393 and name CA)	8.91	0.14	0.13
	assign (segid 3A4 and resid 390 and name CA) (segid 3A4 and resid 393 and name N)	7.68	0.10	0.11
	assign (segid 3A4 and resid 390 and name CA) (segid 3A4 and resid 394 and name CA)	8.28	0.20	0.21
25	assign (segid 3A4 and resid 390 and name CA) (segid 3A4 and resid 394 and name CB)	7.32	0.23	0.23
	assign (segid 3A4 and resid 390 and name CA) (segid 3A4 and resid 395 and name CA)	11.33	0.25	0.26
	assign (segid 3A4 and resid 390 and name CA) (segid 3A4 and resid 396 and name CA)	13.37	0.24	0.24
	assign (segid 3A4 and resid 390 and name CA) (segid 3A4 and resid 396 and name CB)	13.35	0.35	0.35
	assign (segid 3A4 and resid 390 and name CA) (segid 3A4 and resid 397 and name CA)	12.85	0.16	0.17
30	assign (segid 3A4 and resid 390 and name CA) (segid 3A4 and resid 397 and name CB)	11.69	0.16	0.17
	assign (segid 3A4 and resid 390 and name CA) (segid 3A4 and resid 398 and name CA)	14.02	0.21	0.20
	assign (segid 3A4 and resid 390 and name CA) (segid 3A4 and resid 398 and name CB)	13.45	0.22	0.23
	assign (segid 3A4 and resid 390 and name CA) (segid 3A4 and resid 399 and name CA)	16.81	0.21	0.22
35	assign (segid 3A4 and resid 390 and name CA) (segid 3A4 and resid 399 and name CB)	16.83	0.26	0.26
	assign (segid 3A4 and resid 390 and name CA) (segid 3A4 and resid 400 and name CA)	18.07	0.14	0.15
	assign (segid 3A4 and resid 390 and name CA) (segid 3A4 and resid 400 and name CB)	17.48	0.18	0.19
	assign (segid 3A4 and resid 390 and name CA) (segid 3A4 and resid 401 and name CA)	18.19	0.12	0.12
	assign (segid 3A4 and resid 390 and name CA) (segid 3A4 and resid 402 and name CB)	19.48	0.21	0.22
	assign (segid 3A4 and resid 390 and name CA) (segid 3A4 and resid 433 and name CA)	18.77	0.33	0.33
40	assign (segid 3A4 and resid 390 and name CA) (segid HEM and resid 1 and name C1A)	5.77	0.21	0.20
	assign (segid 3A4 and resid 390 and name CA) (segid HEM and resid 1 and name C2A)	5.65	0.20	0.20
	assign (segid 3A4 and resid 390 and name CA) (segid HEM and resid 1 and name C3A)	6.32	0.13	0.13
	assign (segid 3A4 and resid 390 and name CA) (segid HEM and resid 1 and name C3D)	6.86	0.19	0.20
	assign (segid 3A4 and resid 390 and name CA) (segid HEM and resid 1 and name C4A)	6.77	0.12	0.13
45	assign (segid 3A4 and resid 390 and name CA) (segid HEM and resid 1 and name C4D)	6.40	0.19	0.18
	assign (segid 3A4 and resid 390 and name CA) (segid HEM and resid 1 and name CAA)	5.38	0.28	0.28
	assign (segid 3A4 and resid 390 and name CA) (segid HEM and resid 1 and name CAD)	6.68	0.21	0.22
	assign (segid 3A4 and resid 390 and name CA) (segid HEM and resid 1 and name CBA)	5.50	0.86	0.86
	assign (segid 3A4 and resid 390 and name CA) (segid HEM and resid 1 and name CBD)	5.74	0.14	0.14
50	assign (segid 3A4 and resid 390 and name CA) (segid HEM and resid 1 and name CGA)	5.63	0.92	0.92
	assign (segid 3A4 and resid 390 and name CA) (segid HEM and resid 1 and name CGD)	6.04	0.10	0.10
	assign (segid 3A4 and resid 390 and name CA) (segid HEM and resid 1 and name CHA)	5.72	0.26	0.27
	assign (segid 3A4 and resid 390 and name CA) (segid HEM and resid 1 and name CHB)	7.73	0.15	0.15
	assign (segid 3A4 and resid 390 and name CA) (segid HEM and resid 1 and name CMA)	6.93	0.14	0.14
55	assign (segid 3A4 and resid 390 and name CA) (segid HEM and resid 1 and name FE)	7.52	0.18	0.17
	assign (segid 3A4 and resid 390 and name CA) (segid HEM and resid 1 and name NA)	6.48	0.13	0.13
	assign (segid 3A4 and resid 390 and name CA) (segid HEM and resid 1 and name ND)	7.16	0.16	0.15
	assign (segid 3A4 and resid 390 and name CA) (segid HEM and resid 1 and name O1A)	5.55	0.60	0.59
	assign (segid 3A4 and resid 390 and name CA) (segid HEM and resid 1 and name O1D)	6.21	0.24	0.25
60	assign (segid 3A4 and resid 390 and name CA) (segid HEM and resid 1 and name O2D)	6.42	0.38	0.38
	assign (segid 3A4 and resid 390 and name CB) (segid 3A4 and resid 391 and name C)	4.92	0.14	0.14
	assign (segid 3A4 and resid 390 and name CB) (segid 3A4 and resid 391 and name CA)	4.60	0.11	0.12
	assign (segid 3A4 and resid 390 and name CB) (segid 3A4 and resid 391 and name CB)	5.48	0.14	0.13
	assign (segid 3A4 and resid 390 and name CB) (segid 3A4 and resid 391 and name N)	3.28	0.13	0.13
65	assign (segid 3A4 and resid 390 and name CB) (segid 3A4 and resid 391 and name O)	4.76	0.30	0.30
	assign (segid 3A4 and resid 390 and name CB) (segid 3A4 and resid 392 and name C)	7.67	0.17	0.17
	assign (segid 3A4 and resid 390 and name CB) (segid 3A4 and resid 392 and name CA)	6.67	0.12	0.11
	assign (segid 3A4 and resid 390 and name CB) (segid 3A4 and resid 392 and name CB)	7.64	0.12	0.12
	assign (segid 3A4 and resid 390 and name CB) (segid 3A4 and resid 392 and name N)	5.84	0.11	0.12
70	assign (segid 3A4 and resid 390 and name CB) (segid 3A4 and resid 393 and name CA)	9.26	0.20	0.21
	assign (segid 3A4 and resid 390 and name CB) (segid 3A4 and resid 394 and name CA)	8.19	0.33	0.33
	assign (segid 3A4 and resid 390 and name CB) (segid 3A4 and resid 394 and name CB)	7.04	0.35	0.34
	assign (segid 3A4 and resid 390 and name CB) (segid 3A4 and resid 395 and name CA)	10.95	0.36	0.35
	assign (segid 3A4 and resid 390 and name CB) (segid 3A4 and resid 396 and name CA)	13.36	0.31	0.31
75	assign (segid 3A4 and resid 390 and name CB) (segid 3A4 and resid 396 and name CB)	13.47	0.36	0.37
	assign (segid 3A4 and resid 390 and name CB) (segid 3A4 and resid 397 and name CA)	13.00	0.27	0.28
	assign (segid 3A4 and resid 390 and name CB) (segid 3A4 and resid 397 and name CB)	11.91	0.26	0.26
	assign (segid 3A4 and resid 390 and name CB) (segid 3A4 and resid 398 and name CA)	13.78	0.32	0.31
	assign (segid 3A4 and resid 390 and name CB) (segid 3A4 and resid 398 and name CB)	13.07	0.34	0.34
80	assign (segid 3A4 and resid 390 and name CB) (segid 3A4 and resid 399 and name CA)	16.56	0.32	0.32
	assign (segid 3A4 and resid 390 and name CB) (segid 3A4 and resid 399 and name CB)	16.58	0.36	0.36
	assign (segid 3A4 and resid 390 and name CB) (segid 3A4 and resid 400 and name CA)	18.12	0.28	0.28

	assign (segid 3A4 and resid 390 and name CB)	(segid 3A4 and resid 400 and name CB)	17.65	0.33	0.33
	assign (segid 3A4 and resid 390 and name CB)	(segid 3A4 and resid 401 and name CA)	18.19	0.24	0.24
	assign (segid 3A4 and resid 390 and name CB)	(segid 3A4 and resid 402 and name CB)	19.12	0.32	0.31
	assign (segid 3A4 and resid 390 and name CB)	(segid HEM and resid 1 and name C1A)	7.06	0.22	0.22
5	assign (segid 3A4 and resid 390 and name CB)	(segid HEM and resid 1 and name C2A)	6.94	0.22	0.22
	assign (segid 3A4 and resid 390 and name CB)	(segid HEM and resid 1 and name C3A)	7.44	0.19	0.20
	assign (segid 3A4 and resid 390 and name CB)	(segid HEM and resid 1 and name C4D)	7.68	0.19	0.19
	assign (segid 3A4 and resid 390 and name CB)	(segid HEM and resid 1 and name CAA)	6.75	0.27	0.28
	assign (segid 3A4 and resid 390 and name CB)	(segid HEM and resid 1 and name CBD)	6.99	0.17	0.18
	assign (segid 3A4 and resid 390 and name CB)	(segid HEM and resid 1 and name CGD)	7.27	0.14	0.13
10	assign (segid 3A4 and resid 390 and name CB)	(segid HEM and resid 1 and name CHA)	7.10	0.26	0.25
	assign (segid 3A4 and resid 390 and name CB)	(segid HEM and resid 1 and name NA)	7.61	0.19	0.19
	assign (segid 3A4 and resid 390 and name CB)	(segid HEM and resid 1 and name O1A)	6.81	0.68	0.67
	assign (segid 3A4 and resid 390 and name CB)	(segid HEM and resid 1 and name O1D)	7.32	0.30	0.31
	assign (segid 3A4 and resid 390 and name CB)	(segid 3A4 and resid 390 and name C)	2.41	0.03	0.03
15	assign (segid 3A4 and resid 390 and name N)	(segid 3A4 and resid 390 and name CA)	1.46	0.02	0.01
	assign (segid 3A4 and resid 390 and name N)	(segid 3A4 and resid 390 and name CB)	2.42	0.03	0.04
	assign (segid 3A4 and resid 390 and name N)	(segid 3A4 and resid 390 and name O)	2.72	0.12	0.11
	assign (segid 3A4 and resid 390 and name N)	(segid 3A4 and resid 391 and name C)	5.28	0.09	0.09
	assign (segid 3A4 and resid 390 and name N)	(segid 3A4 and resid 391 and name CA)	4.76	0.03	0.02
20	assign (segid 3A4 and resid 390 and name N)	(segid 3A4 and resid 391 and name CB)	5.95	0.05	0.05
	assign (segid 3A4 and resid 390 and name N)	(segid 3A4 and resid 391 and name NA)	3.55	0.04	0.04
	assign (segid 3A4 and resid 390 and name N)	(segid 3A4 and resid 391 and name O)	5.61	0.29	0.29
	assign (segid 3A4 and resid 390 and name N)	(segid 3A4 and resid 392 and name CA)	6.75	0.16	0.17
	assign (segid 3A4 and resid 390 and name N)	(segid 3A4 and resid 392 and name CB)	7.29	0.17	0.17
25	assign (segid 3A4 and resid 390 and name N)	(segid 3A4 and resid 392 and name NA)	5.81	0.17	0.16
	assign (segid 3A4 and resid 390 and name N)	(segid 3A4 and resid 392 and name O)	6.30	0.23	0.23
	assign (segid 3A4 and resid 390 and name N)	(segid HEM and resid 1 and name C1A)	6.17	0.24	0.23
	assign (segid 3A4 and resid 390 and name N)	(segid HEM and resid 1 and name C2A)	7.04	0.16	0.15
	assign (segid 3A4 and resid 390 and name N)	(segid HEM and resid 1 and name C3D)	6.91	0.22	0.21
30	assign (segid 3A4 and resid 390 and name N)	(segid HEM and resid 1 and name C4A)	7.62	0.11	0.10
	assign (segid 3A4 and resid 390 and name N)	(segid HEM and resid 1 and name C4D)	6.68	0.20	0.20
	assign (segid 3A4 and resid 390 and name N)	(segid HEM and resid 1 and name CAA)	5.60	0.34	0.34
	assign (segid 3A4 and resid 390 and name N)	(segid HEM and resid 1 and name CAD)	6.41	0.25	0.24
	assign (segid 3A4 and resid 390 and name N)	(segid HEM and resid 1 and name CBA)	5.59	0.76	0.77
35	assign (segid 3A4 and resid 390 and name N)	(segid HEM and resid 1 and name CBD)	5.32	0.17	0.18
	assign (segid 3A4 and resid 390 and name N)	(segid HEM and resid 1 and name CGA)	5.41	0.84	0.84
	assign (segid 3A4 and resid 390 and name N)	(segid HEM and resid 1 and name CGD)	5.26	0.14	0.14
	assign (segid 3A4 and resid 390 and name N)	(segid HEM and resid 1 and name CHA)	6.02	0.30	0.30
	assign (segid 3A4 and resid 390 and name N)	(segid HEM and resid 1 and name CMA)	7.66	0.12	0.12
40	assign (segid 3A4 and resid 390 and name N)	(segid HEM and resid 1 and name NA)	7.23	0.14	0.13
	assign (segid 3A4 and resid 390 and name N)	(segid HEM and resid 1 and name O1A)	5.23	0.53	0.52
	assign (segid 3A4 and resid 390 and name N)	(segid HEM and resid 1 and name O1D)	5.32	0.23	0.23
	assign (segid 3A4 and resid 390 and name N)	(segid HEM and resid 1 and name O2A)	5.84	1.32	1.33
	assign (segid 3A4 and resid 390 and name N)	(segid HEM and resid 1 and name O2D)	5.55	0.42	0.43
45	assign (segid 3A4 and resid 390 and name O)	(segid 3A4 and resid 390 and name CB)	3.20	0.08	0.08
	assign (segid 3A4 and resid 390 and name O)	(segid 3A4 and resid 391 and name C)	2.81	0.05	0.05
	assign (segid 3A4 and resid 390 and name O)	(segid 3A4 and resid 391 and name CA)	2.78	0.03	0.03
	assign (segid 3A4 and resid 390 and name O)	(segid 3A4 and resid 391 and name CB)	4.25	0.03	0.02
50	assign (segid 3A4 and resid 390 and name O)	(segid 3A4 and resid 391 and name NA)	2.24	0.00	0.01
	assign (segid 3A4 and resid 390 and name O)	(segid 3A4 and resid 391 and name O)	3.29	0.19	0.19
	assign (segid 3A4 and resid 390 and name O)	(segid 3A4 and resid 392 and name C)	5.37	0.15	0.15
	assign (segid 3A4 and resid 390 and name O)	(segid 3A4 and resid 392 and name CA)	4.10	0.11	0.11
	assign (segid 3A4 and resid 390 and name O)	(segid 3A4 and resid 392 and name CB)	4.75	0.09	0.08
	assign (segid 3A4 and resid 390 and name O)	(segid 3A4 and resid 392 and name NA)	3.18	0.13	0.13
55	assign (segid 3A4 and resid 390 and name O)	(segid 3A4 and resid 392 and name O)	6.17	0.21	0.21
	assign (segid 3A4 and resid 390 and name O)	(segid 3A4 and resid 393 and name C)	7.51	0.18	0.19
	assign (segid 3A4 and resid 390 and name O)	(segid 3A4 and resid 393 and name CA)	7.17	0.15	0.15
	assign (segid 3A4 and resid 390 and name O)	(segid 3A4 and resid 393 and name NA)	5.82	0.13	0.13
	assign (segid 3A4 and resid 390 and name O)	(segid 3A4 and resid 394 and name CA)	7.43	0.19	0.20
60	assign (segid 3A4 and resid 390 and name O)	(segid 3A4 and resid 394 and name CB)	6.77	0.22	0.22
	assign (segid 3A4 and resid 390 and name O)	(segid 3A4 and resid 394 and name NA)	6.73	0.18	0.18
	assign (segid 3A4 and resid 390 and name O)	(segid HEM and resid 1 and name C1A)	5.46	0.23	0.23
	assign (segid 3A4 and resid 390 and name O)	(segid HEM and resid 1 and name C1D)	6.30	0.19	0.19
65	assign (segid 3A4 and resid 390 and name O)	(segid HEM and resid 1 and name C2A)	5.92	0.23	0.24
	assign (segid 3A4 and resid 390 and name O)	(segid HEM and resid 1 and name C2D)	6.05	0.23	0.22
	assign (segid 3A4 and resid 390 and name O)	(segid HEM and resid 1 and name C3A)	6.77	0.20	0.20
	assign (segid 3A4 and resid 390 and name O)	(segid HEM and resid 1 and name C3D)	5.30	0.27	0.27
	assign (segid 3A4 and resid 390 and name O)	(segid HEM and resid 1 and name C4A)	6.84	0.19	0.20
	assign (segid 3A4 and resid 390 and name O)	(segid HEM and resid 1 and name C4D)	5.15	0.27	0.26
70	assign (segid 3A4 and resid 390 and name O)	(segid HEM and resid 1 and name CAA)	5.96	0.27	0.28
	assign (segid 3A4 and resid 390 and name O)	(segid HEM and resid 1 and name CAD)	5.21	0.31	0.30
	assign (segid 3A4 and resid 390 and name O)	(segid HEM and resid 1 and name CBA)	6.21	0.64	0.64
	assign (segid 3A4 and resid 390 and name O)	(segid HEM and resid 1 and name CBD)	4.10	0.26	0.26
	assign (segid 3A4 and resid 390 and name O)	(segid HEM and resid 1 and name CGA)	6.60	0.70	0.70
75	assign (segid 3A4 and resid 390 and name O)	(segid HEM and resid 1 and name CGD)	4.70	0.22	0.22
	assign (segid 3A4 and resid 390 and name O)	(segid HEM and resid 1 and name CHA)	4.98	0.30	0.30
	assign (segid 3A4 and resid 390 and name O)	(segid HEM and resid 1 and name CHD)	7.30	0.15	0.15
	assign (segid 3A4 and resid 390 and name O)	(segid HEM and resid 1 and name CMD)	6.92	0.21	0.20
	assign (segid 3A4 and resid 390 and name O)	(segid HEM and resid 1 and name FE)	6.59	0.16	0.16
80	assign (segid 3A4 and resid 390 and name O)	(segid HEM and resid 1 and name NA)	6.10	0.18	0.18
	assign (segid 3A4 and resid 390 and name O)	(segid HEM and resid 1 and name NC)	7.70	0.13	0.13
	assign (segid 3A4 and resid 390 and name O)	(segid HEM and resid 1 and name ND)	5.82	0.20	0.20

	assign (segid 3A4 and resid 390 and name O)	(segid HEM and resid 1 and name O1A)	6.67	0.45	0.46
	assign (segid 3A4 and resid 390 and name O)	(segid HEM and resid 1 and name O1D)	4.85	0.34	0.31
	assign (segid 3A4 and resid 390 and name O)	(segid HEM and resid 1 and name O2D)	5.38	0.47	0.47
	assign (segid 3A4 and resid 391 and name C)	(segid 3A4 and resid 391 and name CB)	2.47	0.02	0.03
5	assign (segid 3A4 and resid 391 and name C)	(segid 3A4 and resid 391 and name O)	1.23	0.01	0.01
	assign (segid 3A4 and resid 391 and name C)	(segid 3A4 and resid 392 and name C)	3.10	0.11	0.12
	assign (segid 3A4 and resid 391 and name C)	(segid 3A4 and resid 392 and name CA)	2.44	0.02	0.01
	assign (segid 3A4 and resid 391 and name C)	(segid 3A4 and resid 392 and name CB)	3.69	0.05	0.06
	assign (segid 3A4 and resid 391 and name C)	(segid 3A4 and resid 392 and name N)	1.33	0.01	0.01
10	assign (segid 3A4 and resid 391 and name C)	(segid 3A4 and resid 392 and name O)	4.04	0.12	0.12
	assign (segid 3A4 and resid 391 and name C)	(segid 3A4 and resid 393 and name C)	4.74	0.19	0.18
	assign (segid 3A4 and resid 391 and name C)	(segid 3A4 and resid 393 and name CA)	4.50	0.17	0.17
	assign (segid 3A4 and resid 391 and name C)	(segid 3A4 and resid 393 and name N)	3.27	0.14	0.13
	assign (segid 3A4 and resid 391 and name C)	(segid 3A4 and resid 393 and name O)	5.93	0.19	0.19
15	assign (segid 3A4 and resid 391 and name C)	(segid 3A4 and resid 394 and name C)	6.23	0.08	0.09
	assign (segid 3A4 and resid 391 and name C)	(segid 3A4 and resid 394 and name CA)	4.88	0.09	0.10
	assign (segid 3A4 and resid 391 and name C)	(segid 3A4 and resid 394 and name CB)	4.57	0.05	0.06
	assign (segid 3A4 and resid 391 and name C)	(segid 3A4 and resid 394 and name N)	4.02	0.13	0.13
	assign (segid 3A4 and resid 391 and name C)	(segid 3A4 and resid 394 and name O)	7.26	0.09	0.09
20	assign (segid 3A4 and resid 391 and name C)	(segid 3A4 and resid 395 and name N)	6.46	0.08	0.09
	assign (segid 3A4 and resid 391 and name C)	(segid HEM and resid 1 and name C1A)	5.12	0.08	0.08
	assign (segid 3A4 and resid 391 and name C)	(segid HEM and resid 1 and name C1B)	6.71	0.08	0.08
	assign (segid 3A4 and resid 391 and name C)	(segid HEM and resid 1 and name C1C)	6.38	0.16	0.17
	assign (segid 3A4 and resid 391 and name C)	(segid HEM and resid 1 and name C1D)	4.94	0.14	0.14
25	assign (segid 3A4 and resid 391 and name C)	(segid HEM and resid 1 and name C2A)	6.01	0.06	0.05
	assign (segid 3A4 and resid 391 and name C)	(segid HEM and resid 1 and name C2B)	7.74	0.09	0.09
	assign (segid 3A4 and resid 391 and name C)	(segid HEM and resid 1 and name C2C)	7.05	0.19	0.18
	assign (segid 3A4 and resid 391 and name C)	(segid HEM and resid 1 and name C2D)	5.27	0.15	0.14
	assign (segid 3A4 and resid 391 and name C)	(segid HEM and resid 1 and name C3A)	6.50	0.06	0.06
30	assign (segid 3A4 and resid 391 and name C)	(segid HEM and resid 1 and name C3B)	7.79	0.12	0.12
	assign (segid 3A4 and resid 391 and name C)	(segid HEM and resid 1 and name C3C)	6.71	0.17	0.17
	assign (segid 3A4 and resid 391 and name C)	(segid HEM and resid 1 and name C3D)	5.03	0.12	0.12
	assign (segid 3A4 and resid 391 and name C)	(segid HEM and resid 1 and name C4A)	5.98	0.08	0.09
	assign (segid 3A4 and resid 391 and name C)	(segid HEM and resid 1 and name C4B)	6.82	0.13	0.13
35	assign (segid 3A4 and resid 391 and name C)	(segid HEM and resid 1 and name C4C)	5.77	0.15	0.14
	assign (segid 3A4 and resid 391 and name C)	(segid HEM and resid 1 and name C4D)	4.58	0.08	0.08
	assign (segid 3A4 and resid 391 and name C)	(segid HEM and resid 1 and name CAA)	6.71	0.09	0.09
	assign (segid 3A4 and resid 391 and name C)	(segid HEM and resid 1 and name CAC)	7.45	0.17	0.16
	assign (segid 3A4 and resid 391 and name C)	(segid HEM and resid 1 and name CAD)	5.70	0.11	0.12
40	assign (segid 3A4 and resid 391 and name C)	(segid HEM and resid 1 and name CBA)	7.20	0.65	0.65
	assign (segid 3A4 and resid 391 and name C)	(segid HEM and resid 1 and name CBD)	5.09	0.08	0.08
	assign (segid 3A4 and resid 391 and name C)	(segid HEM and resid 1 and name CGD)	6.28	0.10	0.10
	assign (segid 3A4 and resid 391 and name C)	(segid HEM and resid 1 and name CHA)	4.87	0.11	0.10
	assign (segid 3A4 and resid 391 and name C)	(segid HEM and resid 1 and name CHB)	6.66	0.11	0.11
45	assign (segid 3A4 and resid 391 and name C)	(segid HEM and resid 1 and name CHC)	6.91	0.16	0.17
	assign (segid 3A4 and resid 391 and name C)	(segid HEM and resid 1 and name CHD)	5.55	0.14	0.14
	assign (segid 3A4 and resid 391 and name C)	(segid HEM and resid 1 and name CMA)	7.72	0.10	0.09
	assign (segid 3A4 and resid 391 and name C)	(segid HEM and resid 1 and name CMD)	6.24	0.17	0.17
	assign (segid 3A4 and resid 391 and name C)	(segid HEM and resid 1 and name FE)	4.85	0.16	0.16
50	assign (segid 3A4 and resid 391 and name C)	(segid HEM and resid 1 and name NA)	5.12	0.07	0.07
	assign (segid 3A4 and resid 391 and name C)	(segid HEM and resid 1 and name NB)	6.10	0.12	0.11
	assign (segid 3A4 and resid 391 and name C)	(segid HEM and resid 1 and name NC)	5.54	0.14	0.15
	assign (segid 3A4 and resid 391 and name C)	(segid HEM and resid 1 and name ND)	4.55	0.11	0.11
	assign (segid 3A4 and resid 391 and name C)	(segid HEM and resid 1 and name O1D)	6.60	0.33	0.33
55	assign (segid 3A4 and resid 391 and name C)	(segid HEM and resid 1 and name O2D)	7.08	0.20	0.20
	assign (segid 3A4 and resid 391 and name CA)	(segid 3A4 and resid 391 and name C)	1.51	0.01	0.01
	assign (segid 3A4 and resid 391 and name CA)	(segid 3A4 and resid 391 and name CB)	1.53	0.02	0.02
	assign (segid 3A4 and resid 391 and name CA)	(segid 3A4 and resid 391 and name O)	2.39	0.01	0.01
	assign (segid 3A4 and resid 391 and name CA)	(segid 3A4 and resid 392 and name C)	4.43	0.08	0.09
60	assign (segid 3A4 and resid 391 and name CA)	(segid 3A4 and resid 392 and name CA)	3.78	0.02	0.02
	assign (segid 3A4 and resid 391 and name CA)	(segid 3A4 and resid 392 and name CB)	4.81	0.07	0.06
	assign (segid 3A4 and resid 391 and name CA)	(segid 3A4 and resid 392 and name N)	2.41	0.02	0.02
	assign (segid 3A4 and resid 391 and name CA)	(segid 3A4 and resid 392 and name O)	5.45	0.10	0.10
	assign (segid 3A4 and resid 391 and name CA)	(segid 3A4 and resid 393 and name C)	5.51	0.15	0.16
65	assign (segid 3A4 and resid 391 and name CA)	(segid 3A4 and resid 393 and name CA)	5.39	0.14	0.14
	assign (segid 3A4 and resid 391 and name CA)	(segid 3A4 and resid 393 and name N)	4.27	0.09	0.10
	assign (segid 3A4 and resid 391 and name CA)	(segid 3A4 and resid 393 and name O)	6.61	0.19	0.18
	assign (segid 3A4 and resid 391 and name CA)	(segid 3A4 and resid 394 and name C)	6.91	0.11	0.10
	assign (segid 3A4 and resid 391 and name CA)	(segid 3A4 and resid 394 and name CA)	5.43	0.10	0.11
70	assign (segid 3A4 and resid 391 and name CA)	(segid 3A4 and resid 394 and name CB)	5.07	0.09	0.08
	assign (segid 3A4 and resid 391 and name CA)	(segid 3A4 and resid 394 and name N)	4.77	0.10	0.11
	assign (segid 3A4 and resid 391 and name CA)	(segid 3A4 and resid 394 and name O)	7.78	0.11	0.11
	assign (segid 3A4 and resid 391 and name CA)	(segid 3A4 and resid 395 and name CA)	8.83	0.12	0.11
	assign (segid 3A4 and resid 391 and name CA)	(segid 3A4 and resid 395 and name N)	7.38	0.11	0.10
75	assign (segid 3A4 and resid 391 and name CA)	(segid 3A4 and resid 396 and name CA)	10.10	0.19	0.19
	assign (segid 3A4 and resid 391 and name CA)	(segid 3A4 and resid 396 and name CB)	9.94	0.36	0.35
	assign (segid 3A4 and resid 391 and name CA)	(segid 3A4 and resid 397 and name CA)	9.48	0.13	0.13
	assign (segid 3A4 and resid 391 and name CA)	(segid 3A4 and resid 397 and name CB)	8.34	0.15	0.14
	assign (segid 3A4 and resid 391 and name CA)	(segid 3A4 and resid 398 and name CA)	11.30	0.13	0.13
80	assign (segid 3A4 and resid 391 and name CA)	(segid 3A4 and resid 398 and name CB)	11.05	0.13	0.14
	assign (segid 3A4 and resid 391 and name CA)	(segid 3A4 and resid 399 and name CA)	13.90	0.12	0.12
	assign (segid 3A4 and resid 391 and name CA)	(segid 3A4 and resid 399 and name CB)	13.88	0.18	0.18
	assign (segid 3A4 and resid 391 and name CA)	(segid 3A4 and resid 400 and name CA)	14.73	0.11	0.11

	assign	(segid 3A4 and resid 391 and name CA)	(segid 3A4 and resid 400 and name CB)	14.01	0.19	0.18
	assign	(segid 3A4 and resid 391 and name CA)	(segid 3A4 and resid 401 and name CA)	15.15	0.10	0.11
	assign	(segid 3A4 and resid 391 and name CA)	(segid 3A4 and resid 402 and name CA)	17.26	0.12	0.13
	assign	(segid 3A4 and resid 391 and name CA)	(segid 3A4 and resid 402 and name CB)	16.92	0.14	0.14
5	assign	(segid 3A4 and resid 391 and name CA)	(segid 3A4 and resid 403 and name CA)	19.29	0.15	0.15
	assign	(segid 3A4 and resid 391 and name CA)	(segid 3A4 and resid 403 and name CB)	18.94	0.17	0.17
	assign	(segid 3A4 and resid 391 and name CA)	(segid 3A4 and resid 404 and name CB)	19.12	0.17	0.18
	assign	(segid 3A4 and resid 391 and name CA)	(segid 3A4 and resid 431 and name CA)	15.85	1.53	1.52
	assign	(segid 3A4 and resid 391 and name CA)	(segid 3A4 and resid 433 and name CA)	16.97	0.40	0.41
10	assign	(segid 3A4 and resid 391 and name CA)	(segid 3A4 and resid 434 and name CA)	18.45	0.46	0.47
	assign	(segid 3A4 and resid 391 and name CA)	(segid HEM and resid 1 and name C1A)	3.79	0.11	0.12
	assign	(segid 3A4 and resid 391 and name CA)	(segid HEM and resid 1 and name C1B)	5.71	0.08	0.08
	assign	(segid 3A4 and resid 391 and name CA)	(segid HEM and resid 1 and name C1C)	6.24	0.14	0.13
	assign	(segid 3A4 and resid 391 and name CA)	(segid HEM and resid 1 and name C1D)	4.76	0.16	0.17
15	assign	(segid 3A4 and resid 391 and name CA)	(segid HEM and resid 1 and name C2A)	4.55	0.06	0.07
	assign	(segid 3A4 and resid 391 and name CA)	(segid HEM and resid 1 and name C2B)	6.85	0.07	0.08
	assign	(segid 3A4 and resid 391 and name CA)	(segid HEM and resid 1 and name C2C)	7.16	0.15	0.15
	assign	(segid 3A4 and resid 391 and name CA)	(segid HEM and resid 1 and name C2D)	5.15	0.17	0.17
	assign	(segid 3A4 and resid 391 and name CA)	(segid HEM and resid 1 and name C3A)	5.04	0.06	0.05
20	assign	(segid 3A4 and resid 391 and name CA)	(segid HEM and resid 1 and name C3B)	7.12	0.09	0.10
	assign	(segid 3A4 and resid 391 and name CA)	(segid HEM and resid 1 and name C3C)	6.91	0.15	0.15
	assign	(segid 3A4 and resid 391 and name CA)	(segid HEM and resid 1 and name C3D)	4.62	0.16	0.16
	assign	(segid 3A4 and resid 391 and name CA)	(segid HEM and resid 1 and name C4A)	4.65	0.09	0.08
	assign	(segid 3A4 and resid 391 and name CA)	(segid HEM and resid 1 and name C4B)	6.24	0.11	0.10
25	assign	(segid 3A4 and resid 391 and name CA)	(segid HEM and resid 1 and name C4C)	5.78	0.13	0.14
	assign	(segid 3A4 and resid 391 and name CA)	(segid HEM and resid 1 and name C4D)	3.85	0.14	0.13
	assign	(segid 3A4 and resid 391 and name CA)	(segid HEM and resid 1 and name CAA)	5.29	0.10	0.10
	assign	(segid 3A4 and resid 391 and name CA)	(segid HEM and resid 1 and name CAD)	5.29	0.15	0.16
	assign	(segid 3A4 and resid 391 and name CA)	(segid HEM and resid 1 and name CBA)	5.82	0.66	0.65
30	assign	(segid 3A4 and resid 391 and name CA)	(segid HEM and resid 1 and name CBD)	4.89	0.10	0.09
	assign	(segid 3A4 and resid 391 and name CA)	(segid HEM and resid 1 and name CGA)	6.78	0.63	0.62
	assign	(segid 3A4 and resid 391 and name CA)	(segid HEM and resid 1 and name CGD)	6.06	0.08	0.08
	assign	(segid 3A4 and resid 391 and name CA)	(segid HEM and resid 1 and name CHA)	3.77	0.17	0.17
	assign	(segid 3A4 and resid 391 and name CA)	(segid HEM and resid 1 and name CHB)	5.44	0.13	0.12
35	assign	(segid 3A4 and resid 391 and name CA)	(segid HEM and resid 1 and name CHC)	6.60	0.13	0.14
	assign	(segid 3A4 and resid 391 and name CA)	(segid HEM and resid 1 and name CHD)	5.59	0.15	0.14
	assign	(segid 3A4 and resid 391 and name CA)	(segid HEM and resid 1 and name CMA)	6.24	0.10	0.09
	assign	(segid 3A4 and resid 391 and name CA)	(segid HEM and resid 1 and name CMB)	7.84	0.05	0.04
	assign	(segid 3A4 and resid 391 and name CA)	(segid HEM and resid 1 and name CMD)	6.38	0.18	0.18
40	assign	(segid 3A4 and resid 391 and name CA)	(segid HEM and resid 1 and name FE)	4.11	0.15	0.16
	assign	(segid 3A4 and resid 391 and name CA)	(segid HEM and resid 1 and name NA)	3.88	0.08	0.08
	assign	(segid 3A4 and resid 391 and name CA)	(segid HEM and resid 1 and name NB)	5.29	0.09	0.10
	assign	(segid 3A4 and resid 391 and name CA)	(segid HEM and resid 1 and name NC)	5.30	0.13	0.12
	assign	(segid 3A4 and resid 391 and name CA)	(segid HEM and resid 1 and name ND)	3.99	0.14	0.14
45	assign	(segid 3A4 and resid 391 and name CA)	(segid HEM and resid 1 and name O1A)	7.06	0.39	0.39
	assign	(segid 3A4 and resid 391 and name CA)	(segid HEM and resid 1 and name O1D)	6.53	0.23	0.22
	assign	(segid 3A4 and resid 391 and name CA)	(segid HEM and resid 1 and name O2D)	6.72	0.16	0.15
	assign	(segid 3A4 and resid 391 and name CB)	(segid 3A4 and resid 392 and name C)	4.85	0.04	0.04
50	assign	(segid 3A4 and resid 391 and name CB)	(segid 3A4 and resid 392 and name CA)	4.66	0.08	0.07
	assign	(segid 3A4 and resid 391 and name CB)	(segid 3A4 and resid 392 and name CB)	5.80	0.	

	assign	(segid 3A4 and resid 391 and name CB)	(segid 3A4 and resid 434 and name CA)	17.20	0.51	0.50
	assign	(segid 3A4 and resid 391 and name CB)	(segid HEM and resid 1 and name C1A)	3.72	0.16	0.16
	assign	(segid 3A4 and resid 391 and name CB)	(segid HEM and resid 1 and name C1B)	4.41	0.09	0.09
	assign	(segid 3A4 and resid 391 and name CB)	(segid HEM and resid 1 and name C1C)	5.36	0.15	0.15
5	assign	(segid 3A4 and resid 391 and name CB)	(segid HEM and resid 1 and name C1D)	4.98	0.16	0.16
	assign	(segid 3A4 and resid 391 and name CB)	(segid HEM and resid 1 and name C2A)	4.43	0.11	0.12
	assign	(segid 3A4 and resid 391 and name CB)	(segid HEM and resid 1 and name C2B)	5.44	0.08	0.08
	assign	(segid 3A4 and resid 391 and name CB)	(segid HEM and resid 1 and name C2C)	6.43	0.15	0.15
	assign	(segid 3A4 and resid 391 and name CB)	(segid HEM and resid 1 and name C2D)	5.73	0.15	0.15
10	assign	(segid 3A4 and resid 391 and name CB)	(segid HEM and resid 1 and name C3A)	4.51	0.06	0.06
	assign	(segid 3A4 and resid 391 and name CB)	(segid HEM and resid 1 and name C3B)	5.71	0.10	0.11
	assign	(segid 3A4 and resid 391 and name CB)	(segid HEM and resid 1 and name C3C)	6.47	0.15	0.14
	assign	(segid 3A4 and resid 391 and name CB)	(segid HEM and resid 1 and name C3D)	5.35	0.15	0.14
	assign	(segid 3A4 and resid 391 and name CB)	(segid HEM and resid 1 and name C4A)	3.82	0.10	0.09
15	assign	(segid 3A4 and resid 391 and name CB)	(segid HEM and resid 1 and name C4B)	4.95	0.10	0.11
	assign	(segid 3A4 and resid 391 and name CB)	(segid HEM and resid 1 and name C4C)	5.42	0.14	0.14
	assign	(segid 3A4 and resid 391 and name CB)	(segid HEM and resid 1 and name C4D)	4.27	0.14	0.14
	assign	(segid 3A4 and resid 391 and name CB)	(segid HEM and resid 1 and name CAA)	5.49	0.13	0.14
	assign	(segid 3A4 and resid 391 and name CB)	(segid HEM and resid 1 and name CAB)	6.85	0.14	0.14
20	assign	(segid 3A4 and resid 391 and name CB)	(segid HEM and resid 1 and name CAC)	7.58	0.16	0.16
	assign	(segid 3A4 and resid 391 and name CB)	(segid HEM and resid 1 and name CAD)	6.27	0.14	0.14
	assign	(segid 3A4 and resid 391 and name CB)	(segid HEM and resid 1 and name CBA)	6.13	0.60	0.60
	assign	(segid 3A4 and resid 391 and name CB)	(segid HEM and resid 1 and name CBD)	6.14	0.10	0.09
	assign	(segid 3A4 and resid 391 and name CB)	(segid HEM and resid 1 and name CGD)	7.39	0.10	0.10
25	assign	(segid 3A4 and resid 391 and name CB)	(segid HEM and resid 1 and name CHA)	4.15	0.17	0.17
	assign	(segid 3A4 and resid 391 and name CB)	(segid HEM and resid 1 and name CHB)	4.30	0.13	0.12
	assign	(segid 3A4 and resid 391 and name CB)	(segid HEM and resid 1 and name CHC)	5.46	0.14	0.14
	assign	(segid 3A4 and resid 391 and name CB)	(segid HEM and resid 1 and name CHD)	5.58	0.14	0.15
	assign	(segid 3A4 and resid 391 and name CB)	(segid HEM and resid 1 and name CMA)	5.65	0.07	0.07
30	assign	(segid 3A4 and resid 391 and name CB)	(segid HEM and resid 1 and name CMB)	6.41	0.04	0.04
	assign	(segid 3A4 and resid 391 and name CB)	(segid HEM and resid 1 and name CMC)	7.58	0.14	0.14
	assign	(segid 3A4 and resid 391 and name CB)	(segid HEM and resid 1 and name CMD)	7.07	0.16	0.15
	assign	(segid 3A4 and resid 391 and name CB)	(segid HEM and resid 1 and name FE)	3.39	0.18	0.18
	assign	(segid 3A4 and resid 391 and name CB)	(segid HEM and resid 1 and name NA)	3.29	0.13	0.13
35	assign	(segid 3A4 and resid 391 and name CB)	(segid HEM and resid 1 and name NB)	4.09	0.10	0.11
	assign	(segid 3A4 and resid 391 and name CB)	(segid HEM and resid 1 and name NC)	4.64	0.14	0.13
	assign	(segid 3A4 and resid 391 and name CB)	(segid HEM and resid 1 and name ND)	4.03	0.16	0.15
	assign	(segid 3A4 and resid 391 and name N)	(segid 3A4 and resid 391 and name C)	2.45	0.06	0.07
40	assign	(segid 3A4 and resid 391 and name N)	(segid 3A4 and resid 391 and name CA)	1.44	0.01	0.02
	assign	(segid 3A4 and resid 391 and name N)	(segid 3A4 and resid 391 and name CB)	2.42	0.01	0.02
	assign	(segid 3A4 and resid 391 and name N)	(segid 3A4 and resid 391 and name C)	2.94	0.13	0.13
	assign	(segid 3A4 and resid 391 and name N)	(segid 3A4 and resid 392 and name C)	5.55	0.13	0.14
45	assign	(segid 3A4 and resid 391 and name N)	(segid 3A4 and resid 392 and name CA)	4.72	0.08	0.08
	assign	(segid 3A4 and resid 391 and name N)	(segid 3A4 and resid 392 and name CB)	5.73	0.08	0.09
	assign	(segid 3A4 and resid 391 and name N)	(segid 3A4 and resid 392 and name N)	3.45	0.08	0.08
	assign	(segid 3A4 and resid 391 and name N)	(segid 3A4 and resid 392 and name O)	6.45	0.16	0.16
50	assign	(segid 3A4 and resid 391 and name N)	(segid 3A4 and resid 393 and name C)	6.72	0.19	0.19
	assign	(segid 3A4 and resid 391 and name N)	(segid 3A4 and resid 393 and name CA)	6.71	0.16	0.17
	assign	(segid 3A4 and resid 391 and name N)	(segid 3A4 and resid 393 and name N)	5.59	0.13	0.12
	assign	(segid 3A4 and resid 391				

	assign (segid 3A4 and resid 391 and name N)	(segid HEM and resid 1 and name O1D)	6.46	0.23	0.24
	assign (segid 3A4 and resid 391 and name N)	(segid HEM and resid 1 and name O2D)	6.63	0.24	0.24
	assign (segid 3A4 and resid 391 and name O)	(segid 3A4 and resid 391 and name CB)	2.99	0.09	0.10
	assign (segid 3A4 and resid 391 and name O)	(segid 3A4 and resid 392 and name C)	3.16	0.19	0.19
	assign (segid 3A4 and resid 391 and name O)	(segid 3A4 and resid 392 and name CA)	2.77	0.01	0.02
5	assign (segid 3A4 and resid 391 and name O)	(segid 3A4 and resid 392 and name CB)	4.24	0.08	0.07
	assign (segid 3A4 and resid 391 and name O)	(segid 3A4 and resid 392 and name N)	2.25	0.02	0.02
	assign (segid 3A4 and resid 391 and name O)	(segid 3A4 and resid 392 and name O)	3.78	0.23	0.22
	assign (segid 3A4 and resid 391 and name O)	(segid 3A4 and resid 393 and name C)	4.54	0.37	0.36
	assign (segid 3A4 and resid 391 and name O)	(segid 3A4 and resid 393 and name CA)	4.58	0.32	0.32
10	assign (segid 3A4 and resid 391 and name O)	(segid 3A4 and resid 393 and name N)	3.53	0.27	0.27
	assign (segid 3A4 and resid 391 and name O)	(segid 3A4 and resid 393 and name O)	5.71	0.36	0.35
	assign (segid 3A4 and resid 391 and name O)	(segid 3A4 and resid 394 and name C)	5.54	0.29	0.28
	assign (segid 3A4 and resid 391 and name O)	(segid 3A4 and resid 394 and name CA)	4.28	0.30	0.29
	assign (segid 3A4 and resid 391 and name O)	(segid 3A4 and resid 394 and name CB)	3.74	0.22	0.22
15	assign (segid 3A4 and resid 391 and name O)	(segid 3A4 and resid 394 and name N)	3.60	0.36	0.35
	assign (segid 3A4 and resid 391 and name O)	(segid 3A4 and resid 394 and name O)	6.60	0.30	0.30
	assign (segid 3A4 and resid 391 and name O)	(segid 3A4 and resid 395 and name CA)	7.06	0.23	0.23
	assign (segid 3A4 and resid 391 and name O)	(segid 3A4 and resid 395 and name N)	5.68	0.24	0.25
20	assign (segid 3A4 and resid 391 and name O)	(segid HEM and resid 1 and name C1A)	6.13	0.11	0.10
	assign (segid 3A4 and resid 391 and name O)	(segid HEM and resid 1 and name C1B)	7.25	0.18	0.18
	assign (segid 3A4 and resid 391 and name O)	(segid HEM and resid 1 and name C1C)	6.95	0.31	0.32
	assign (segid 3A4 and resid 391 and name O)	(segid HEM and resid 1 and name C1D)	6.03	0.18	0.18
	assign (segid 3A4 and resid 391 and name O)	(segid HEM and resid 1 and name C2A)	6.90	0.07	0.07
	assign (segid 3A4 and resid 391 and name O)	(segid HEM and resid 1 and name C2D)	6.41	0.15	0.15
25	assign (segid 3A4 and resid 391 and name O)	(segid HEM and resid 1 and name C3A)	7.26	0.06	0.07
	assign (segid 3A4 and resid 391 and name O)	(segid HEM and resid 1 and name C3C)	7.35	0.28	0.28
	assign (segid 3A4 and resid 391 and name O)	(segid HEM and resid 1 and name C3D)	6.23	0.11	0.12
	assign (segid 3A4 and resid 391 and name O)	(segid HEM and resid 1 and name C4A)	6.74	0.10	0.10
	assign (segid 3A4 and resid 391 and name O)	(segid HEM and resid 1 and name C4B)	7.29	0.28	0.28
30	assign (segid 3A4 and resid 391 and name O)	(segid HEM and resid 1 and name C4C)	6.57	0.24	0.23
	assign (segid 3A4 and resid 391 and name O)	(segid HEM and resid 1 and name C4D)	5.77	0.08	0.08
	assign (segid 3A4 and resid 391 and name O)	(segid HEM and resid 1 and name CAA)	7.59	0.09	0.09
	assign (segid 3A4 and resid 391 and name O)	(segid HEM and resid 1 and name CAD)	6.87	0.09	0.09
35	assign (segid 3A4 and resid 391 and name O)	(segid HEM and resid 1 and name CBD)	6.16	0.12	0.12
	assign (segid 3A4 and resid 391 and name O)	(segid HEM and resid 1 and name CGD)	7.25	0.18	0.19
	assign (segid 3A4 and resid 391 and name O)	(segid HEM and resid 1 and name CHA)	6.00	0.11	0.11
	assign (segid 3A4 and resid 391 and name O)	(segid HEM and resid 1 and name CHB)	7.26	0.13	0.14
	assign (segid 3A4 and resid 391 and name O)	(segid HEM and resid 1 and name CHD)	6.49	0.21	0.21
40	assign (segid 3A4 and resid 391 and name O)	(segid HEM and resid 1 and name CMD)	7.31	0.18	0.18
	assign (segid 3A4 and resid 391 and name O)	(segid HEM and resid 1 and name FE)	5.73	0.27	0.26
	assign (segid 3A4 and resid 391 and name O)	(segid HEM and resid 1 and name NA)	6.02	0.12	0.13
	assign (segid 3A4 and resid 391 and name O)	(segid HEM and resid 1 and name NB)	6.71	0.21	0.22
	assign (segid 3A4 and resid 391 and name O)	(segid HEM and resid 1 and name NC)	6.30	0.25	0.25
45	assign (segid 3A4 and resid 391 and name O)	(segid HEM and resid 1 and name ND)	5.66	0.15	0.15
	assign (segid 3A4 and resid 392 and name C)	(segid 3A4 and resid 392 and name CB)	2.53	0.05	0.05
	assign (segid 3A4 and resid 392 and name C)	(segid 3A4 and resid 392 and name O)	1.24	0.01	0.00
	assign (segid 3A4 and resid 392 and name C)	(segid 3A4 and resid 393 and name C)	3.30	0.06	0.05
	assign (segid 3A4 and resid 392 and name C)	(segid 3A4 and resid 393 and name CA)	2.42	0.01	0.01
50	assign (segid 3A4 and resid 392 and name C)	(segid 3A4 and resid 393 and name N)	1.32	0.01	0.01
	assign (segid 3A4 and resid 392 and name C)	(segid 3A4 and resid 393 and name O)	4.43	0.08	0.08
	assign (segid 3A4 and resid 392 and name C)	(segid 3A4 and resid 394 and name C)	5.50	0.10	0.11
	assign (segid 3A4 and resid 392 and name C)	(segid 3A4 and resid 394 and name CA)	4.67	0.07	0.08
	assign (segid 3A4 and resid 392 and name C)	(segid 3A4 and resid 394 and name CB)	5.05	0.10	0.10
55	assign (segid 3A4 and resid 392 and name C)	(segid 3A4 and resid 394 and name N)	3.30	0.07	0.07
	assign (segid 3A4 and resid 392 and name C)	(segid 3A4 and resid 394 and name O)	6.65	0.10	0.11
	assign (segid 3A4 and resid 392 and name C)	(segid 3A4 and resid 395 and name C)	6.95	0.10	0.10
	assign (segid 3A4 and resid 392 and name C)	(segid 3A4 and resid 395 and name CA)	6.42	0.14	0.15
	assign (segid 3A4 and resid 392 and name C)	(segid 3A4 and resid 395 and name N)	5.25	0.12	0.13
60	assign (segid 3A4 and resid 392 and name C)	(segid 3A4 and resid 396 and name CA)	7.13	0.14	0.14
	assign (segid 3A4 and resid 392 and name C)	(segid 3A4 and resid 396 and name CB)	6.66	0.27	0.26
	assign (segid 3A4 and resid 392 and name C)	(segid 3A4 and resid 396 and name N)	6.30	0.09	0.08
	assign (segid 3A4 and resid 392 and name C)	(segid 3A4 and resid 397 and name CB)	7.62	0.16	0.16
	assign (segid 3A4 and resid 392 and name C)	(segid 3A4 and resid 397 and name N)	7.22	0.09	0.08
65	assign (segid 3A4 and resid 392 and name C)	(segid HEM and resid 1 and name C1A)	7.34	0.09	0.09
	assign (segid 3A4 and resid 392 and name C)	(segid HEM and resid 1 and name C1C)	6.04	0.21	0.20
	assign (segid 3A4 and resid 392 and name C)	(segid HEM and resid 1 and name C1D)	5.15	0.19	0.18
	assign (segid 3A4 and resid 392 and name C)	(segid HEM and resid 1 and name C2C)	6.04	0.23	0.24
	assign (segid 3A4 and resid 392 and name C)	(segid HEM and resid 1 and name C2D)	5.55	0.21	0.20
70	assign (segid 3A4 and resid 392 and name C)	(segid HEM and resid 1 and name C3C)	5.52	0.25	0.26
	assign (segid 3A4 and resid 392 and name C)	(segid HEM and resid 1 and name C3D)	6.03	0.17	0.17
	assign (segid 3A4 and resid 392 and name C)	(segid HEM and resid 1 and name C4B)	7.40	0.17	0.16
	assign (segid 3A4 and resid 392 and name C)	(segid HEM and resid 1 and name C4C)	5.17	0.24	0.23
	assign (segid 3A4 and resid 392 and name C)	(segid HEM and resid 1 and name C4D)	6.01	0.12	0.11
75	assign (segid 3A4 and resid 392 and name C)	(segid HEM and resid 1 and name CAC)	5.79	0.26	0.25
	assign (segid 3A4 and resid 392 and name C)	(segid HEM and resid 1 and name CAD)	6.91	0.16	0.17
	assign (segid 3A4 and resid 392 and name C)	(segid HEM and resid 1 and name CBC)	6.16	0.43	0.43
	assign (segid 3A4 and resid 392 and name C)	(segid HEM and resid 1 and name CBD)	6.45	0.17	0.16
	assign (segid 3A4 and resid 392 and name C)	(segid HEM and resid 1 and name CGD)	7.72	0.18	0.19
80	assign (segid 3A4 and resid 392 and name C)	(segid HEM and resid 1 and name CHA)	6.87	0.10	0.11
	assign (segid 3A4 and resid 392 and name C)	(segid HEM and resid 1 and name CHC)	6.90	0.19	0.18
	assign (segid 3A4 and resid 392 and name C)	(segid HEM and resid 1 and name CHD)	5.04	0.20	0.21
	assign (segid 3A4 and resid 392 and name C)	(segid HEM and resid 1 and name CMC)	6.92	0.24	0.23

	assign (segid 3A4 and resid 392 and name C) (segid HEM and resid 1 and name CMD)	5.93	0.24	0.25
	assign (segid 3A4 and resid 392 and name C) (segid HEM and resid 1 and name FE)	5.93	0.17	0.17
	assign (segid 3A4 and resid 392 and name C) (segid HEM and resid 1 and name NA)	7.06	0.08	0.09
	assign (segid 3A4 and resid 392 and name C) (segid HEM and resid 1 and name NB)	7.15	0.14	0.14
5	assign (segid 3A4 and resid 392 and name C) (segid HEM and resid 1 and name NC)	5.51	0.21	0.21
	assign (segid 3A4 and resid 392 and name C) (segid HEM and resid 1 and name ND)	5.49	0.14	0.14
	assign (segid 3A4 and resid 392 and name CA) (segid 3A4 and resid 392 and name C)	1.54	0.02	0.01
	assign (segid 3A4 and resid 392 and name CA) (segid 3A4 and resid 392 and name CB)	1.55	0.03	0.03
	assign (segid 3A4 and resid 392 and name CA) (segid 3A4 and resid 392 and name O)	2.40	0.03	0.02
10	assign (segid 3A4 and resid 392 and name CA) (segid 3A4 and resid 393 and name C)	4.63	0.04	0.05
	assign (segid 3A4 and resid 392 and name CA) (segid 3A4 and resid 393 and name CA)	3.80	0.02	0.03
	assign (segid 3A4 and resid 392 and name CA) (segid 3A4 and resid 393 and name N)	2.43	0.01	0.01
	assign (segid 3A4 and resid 392 and name CA) (segid 3A4 and resid 393 and name O)	5.83	0.07	0.07
	assign (segid 3A4 and resid 392 and name CA) (segid 3A4 and resid 394 and name C)	6.66	0.11	0.12
15	assign (segid 3A4 and resid 392 and name CA) (segid 3A4 and resid 394 and name CA)	5.65	0.09	0.09
	assign (segid 3A4 and resid 392 and name CA) (segid 3A4 and resid 394 and name CB)	5.71	0.12	0.12
	assign (segid 3A4 and resid 392 and name CA) (segid 3A4 and resid 394 and name O)	4.40	0.06	0.06
	assign (segid 3A4 and resid 392 and name CA) (segid 3A4 and resid 394 and name N)	7.82	0.12	0.12
	assign (segid 3A4 and resid 392 and name CA) (segid 3A4 and resid 395 and name CA)	7.70	0.17	0.16
20	assign (segid 3A4 and resid 392 and name CA) (segid 3A4 and resid 395 and name N)	6.48	0.15	0.14
	assign (segid 3A4 and resid 392 and name CA) (segid 3A4 and resid 396 and name CA)	8.65	0.13	0.14
	assign (segid 3A4 and resid 392 and name CA) (segid 3A4 and resid 396 and name CB)	8.18	0.27	0.26
	assign (segid 3A4 and resid 392 and name CA) (segid 3A4 and resid 396 and name N)	7.78	0.09	0.08
	assign (segid 3A4 and resid 392 and name CA) (segid 3A4 and resid 397 and name CA)	9.48	0.15	0.15
25	assign (segid 3A4 and resid 392 and name CA) (segid 3A4 and resid 397 and name CB)	8.81	0.20	0.21
	assign (segid 3A4 and resid 392 and name CA) (segid 3A4 and resid 398 and name CA)	11.54	0.12	0.13
	assign (segid 3A4 and resid 392 and name CA) (segid 3A4 and resid 398 and name CB)	11.33	0.12	0.12
	assign (segid 3A4 and resid 392 and name CA) (segid 3A4 and resid 399 and name CA)	13.20	0.05	0.06
	assign (segid 3A4 and resid 392 and name CA) (segid 3A4 and resid 399 and name CB)	12.78	0.10	0.09
30	assign (segid 3A4 and resid 392 and name CA) (segid 3A4 and resid 400 and name CA)	14.27	0.10	0.09
	assign (segid 3A4 and resid 392 and name CA) (segid 3A4 and resid 400 and name CB)	13.54	0.15	0.15
	assign (segid 3A4 and resid 392 and name CA) (segid 3A4 and resid 401 and name CA)	15.59	0.10	0.10
	assign (segid 3A4 and resid 392 and name CA) (segid 3A4 and resid 402 and name CA)	17.44	0.06	0.06
	assign (segid 3A4 and resid 392 and name CA) (segid 3A4 and resid 402 and name CB)	16.96	0.07	0.08
35	assign (segid 3A4 and resid 392 and name CA) (segid 3A4 and resid 403 and name CA)	18.88	0.12	0.12
	assign (segid 3A4 and resid 392 and name CA) (segid 3A4 and resid 403 and name CB)	18.26	0.13	0.14
	assign (segid 3A4 and resid 392 and name CA) (segid 3A4 and resid 404 and name CB)	19.26	0.26	0.26
	assign (segid 3A4 and resid 392 and name CA) (segid HEM and resid 1 and name C1A)	6.78	0.07	0.07
	assign (segid 3A4 and resid 392 and name CA) (segid HEM and resid 1 and name C1C)	6.78	0.19	0.19
40	assign (segid 3A4 and resid 392 and name CA) (segid HEM and resid 1 and name C1D)	4.94	0.14	0.13
	assign (segid 3A4 and resid 392 and name CA) (segid HEM and resid 1 and name C2C)	6.97	0.19	0.19
	assign (segid 3A4 and resid 392 and name CA) (segid HEM and resid 1 and name C2D)	5.00	0.15	0.14
	assign (segid 3A4 and resid 392 and name CA) (segid HEM and resid 1 and name C3C)	6.31	0.21	0.21
	assign (segid 3A4 and resid 392 and name CA) (segid HEM and resid 1 and name C3D)	5.24	0.12	0.11
45	assign (segid 3A4 and resid 392 and name CA) (segid HEM and resid 1 and name C4C)	5.66	0.23	0.22
	assign (segid 3A4 and resid 392 and name CA) (segid HEM and resid 1 and name C4D)	5.37	0.09	0.10
	assign (segid 3A4 and resid 392 and name CA) (segid HEM and resid 1 and name CAC)	6.59	0.19	0.19
	assign (segid 3A4 and resid 392 and name CA) (segid HEM and resid 1 and name CAD)	5.86	0.13	0.12
	assign (segid 3A4 and resid 392 and name CA) (segid HEM and resid 1 and name CBD)	7.12	0.42	0.41
50	assign (segid 3A4 and resid 392 and name CA) (segid HEM and resid 1 and name CGD)	5.16	0.15	0.16
	assign (segid 3A4 and resid 392 and name CA) (segid HEM and resid 1 and name CHA)	6.34	0.19	0.19
	assign (segid 3A4 and resid 392 and name CA) (segid HEM and resid 1 and name CHB)	6.14	0.06	0.07
	assign (segid 3A4 and resid 392 and name CA) (segid HEM and resid 1 and name CHC)	7.66	0.18	0.17
	assign (segid 3A4 and resid 392 and name CA) (segid HEM and resid 1 and name CHD)	5.21	0.18	0.18
55	assign (segid 3A4 and resid 392 and name CA) (segid HEM and resid 1 and name CMD)	5.40	0.19	0.19
	assign (segid 3A4 and resid 392 and name CA) (segid HEM and resid 1 and name FE)	6.00	0.13	0.14
	assign (segid 3A4 and resid 392 and name CA) (segid HEM and resid 1 and name NA)	6.79	0.10	0.10
	assign (segid 3A4 and resid 392 and name CA) (segid HEM and resid 1 and name NB)	7.48	0.17	0.16
	assign (segid 3A4 and resid 392 and name CA) (segid HEM and resid 1 and name NC)	5.98	0.20	0.20
60	assign (segid 3A4 and resid 392 and name CA) (segid HEM and resid 1 and name ND)	5.21	0.14	0.13
	assign (segid 3A4 and resid 392 and name CA) (segid HEM and resid 1 and name O1D)	6.48	0.44	0.45
	assign (segid 3A4 and resid 392 and name CA) (segid HEM and resid 1 and name O2D)	7.28	0.30	0.29
	assign (segid 3A4 and resid 392 and name CB) (segid 3A4 and resid 393 and name C)	5.69	0.07	0.07
	assign (segid 3A4 and resid 392 and name CB) (segid 3A4 and resid 393 and name CA)	4.55	0.07	0.06
65	assign (segid 3A4 and resid 392 and name CB) (segid 3A4 and resid 393 and name N)	3.26	0.04	0.04
	assign (segid 3A4 and resid 392 and name CB) (segid 3A4 and resid 393 and name O)	6.81	0.09	0.08
	assign (segid 3A4 and resid 392 and name CB) (segid 3A4 and resid 394 and name CA)	7.05	0.09	0.09
	assign (segid 3A4 and resid 392 and name CB) (segid 3A4 and resid 394 and name CB)	7.22	0.11	0.11
	assign (segid 3A4 and resid 392 and name CB) (segid 3A4 and resid 394 and name N)	5.71	0.08	0.08
70	assign (segid 3A4 and resid 392 and name CB) (segid 3A4 and resid 395 and name CA)	8.88	0.18	0.18
	assign (segid 3A4 and resid 392 and name CB) (segid 3A4 and resid 396 and name CA)	9.43	0.12	0.12
	assign (segid 3A4 and resid 392 and name CB) (segid 3A4 and resid 396 and name CB)	8.73	0.25	0.25
	assign (segid 3A4 and resid 392 and name CB) (segid 3A4 and resid 397 and name CA)	10.45	0.18	0.19
	assign (segid 3A4 and resid 392 and name CB) (segid 3A4 and resid 397 and name CB)	9.85	0.25	0.24
75	assign (segid 3A4 and resid 392 and name CB) (segid 3A4 and resid 398 and name CA)	12.78	0.13	0.13
	assign (segid 3A4 and resid 392 and name CB) (segid 3A4 and resid 398 and name CB)	12.65	0.12	0.13
	assign (segid 3A4 and resid 392 and name CB) (segid 3A4 and resid 399 and name CA)	14.21	0.06	0.06
	assign (segid 3A4 and resid 392 and name CB) (segid 3A4 and resid 399 and name CB)	13.69	0.09	0.09
	assign (segid 3A4 and resid 392 and name CB) (segid 3A4 and resid 400 and name CA)	15.08	0.12	0.11
80	assign (segid 3A4 and resid 392 and name CB) (segid 3A4 and resid 400 and name CB)	14.27	0.16	0.16
	assign (segid 3A4 and resid 392 and name CB) (segid 3A4 and resid 401 and name CA)	16.62	0.15	0.14
	assign (segid 3A4 and resid 392 and name CB) (segid 3A4 and resid 402 and name CA)	18.57	0.08	0.09
	assign (segid 3A4 and resid 392 and name CB) (segid 3A4 and resid 402 and name CB)	18.14	0.09	0.09

assign (segid 3A4 and resid 392 and name CB) (segid 3A4 and resid 403 and name CA) 19.81 0.13 0.13
 assign (segid 3A4 and resid 392 and name CB) (segid 3A4 and resid 403 and name CB) 19.11 0.14 0.13
 assign (segid 3A4 and resid 392 and name CB) (segid HEM and resid 1 and name C1A) 7.21 0.13 0.13
 assign (segid 3A4 and resid 392 and name CB) (segid HEM and resid 1 and name C1C) 7.26 0.25 0.25
 5 assign (segid 3A4 and resid 392 and name CB) (segid HEM and resid 1 and name C1D) 4.71 0.20 0.20
 assign (segid 3A4 and resid 392 and name CB) (segid HEM and resid 1 and name C2C) 7.28 0.24 0.24
 assign (segid 3A4 and resid 392 and name CB) (segid HEM and resid 1 and name C2D) 4.41 0.19 0.19
 assign (segid 3A4 and resid 392 and name CB) (segid HEM and resid 1 and name C3C) 6.37 0.26 0.26
 assign (segid 3A4 and resid 392 and name CB) (segid HEM and resid 1 and name C3D) 4.83 0.16 0.16
 10 assign (segid 3A4 and resid 392 and name CB) (segid HEM and resid 1 and name C4C) 5.73 0.29 0.29
 assign (segid 3A4 and resid 392 and name CB) (segid HEM and resid 1 and name C4D) 5.36 0.16 0.17
 assign (segid 3A4 and resid 392 and name CB) (segid HEM and resid 1 and name CAC) 6.38 0.22 0.22
 assign (segid 3A4 and resid 392 and name CB) (segid HEM and resid 1 and name CAD) 5.28 0.15 0.15
 assign (segid 3A4 and resid 392 and name CB) (segid HEM and resid 1 and name CBC) 6.88 0.44 0.44
 15 assign (segid 3A4 and resid 392 and name CB) (segid HEM and resid 1 and name CBD) 4.61 0.17 0.18
 assign (segid 3A4 and resid 392 and name CB) (segid HEM and resid 1 and name CGD) 5.72 0.22 0.21
 assign (segid 3A4 and resid 392 and name CB) (segid HEM and resid 1 and name CHA) 6.32 0.11 0.11
 assign (segid 3A4 and resid 392 and name CB) (segid HEM and resid 1 and name CHD) 4.98 0.26 0.26
 assign (segid 3A4 and resid 392 and name CB) (segid HEM and resid 1 and name CMD) 4.41 0.22 0.22
 20 assign (segid 3A4 and resid 392 and name CB) (segid HEM and resid 1 and name FE) 6.53 0.19 0.19
 assign (segid 3A4 and resid 392 and name CB) (segid HEM and resid 1 and name NA) 7.37 0.17 0.16
 assign (segid 3A4 and resid 392 and name CB) (segid HEM and resid 1 and name NC) 6.35 0.26 0.27
 assign (segid 3A4 and resid 392 and name CB) (segid HEM and resid 1 and name ND) 5.31 0.21 0.20
 assign (segid 3A4 and resid 392 and name CB) (segid HEM and resid 1 and name O1D) 5.81 0.48 0.48
 25 assign (segid 3A4 and resid 392 and name CB) (segid HEM and resid 1 and name O2D) 6.69 0.29 0.28
 assign (segid 3A4 and resid 392 and name N) (segid 3A4 and resid 392 and name C) 2.45 0.03 0.03
 assign (segid 3A4 and resid 392 and name N) (segid 3A4 and resid 392 and name CA) 1.46 0.01 0.01
 assign (segid 3A4 and resid 392 and name N) (segid 3A4 and resid 392 and name CB) 2.45 0.04 0.04
 assign (segid 3A4 and resid 392 and name N) (segid 3A4 and resid 392 and name O) 3.54 0.02 0.01
 30 assign (segid 3A4 and resid 392 and name N) (segid 3A4 and resid 393 and name C) 4.79 0.06 0.06
 assign (segid 3A4 and resid 392 and name N) (segid 3A4 and resid 393 and name CA) 4.14 0.04 0.04
 assign (segid 3A4 and resid 392 and name N) (segid 3A4 and resid 393 and name N) 2.72 0.03 0.03
 assign (segid 3A4 and resid 392 and name N) (segid 3A4 and resid 393 and name O) 6.00 0.06 0.06
 35 assign (segid 3A4 and resid 392 and name N) (segid 3A4 and resid 394 and name C) 6.77 0.13 0.12
 assign (segid 3A4 and resid 392 and name N) (segid 3A4 and resid 394 and name CA) 5.52 0.12 0.12
 assign (segid 3A4 and resid 392 and name N) (segid 3A4 and resid 394 and name CB) 5.47 0.12 0.13
 assign (segid 3A4 and resid 392 and name N) (segid 3A4 and resid 394 and name N) 4.39 0.10 0.09
 assign (segid 3A4 and resid 392 and name N) (segid 3A4 and resid 394 and name O) 7.84 0.13 0.14
 40 assign (segid 3A4 and resid 392 and name N) (segid 3A4 and resid 395 and name N) 6.86 0.14 0.13
 assign (segid 3A4 and resid 392 and name N) (segid HEM and resid 1 and name C1A) 5.38 0.05 0.05
 assign (segid 3A4 and resid 392 and name N) (segid HEM and resid 1 and name C1B) 7.24 0.16 0.15
 assign (segid 3A4 and resid 392 and name N) (segid HEM and resid 1 and name C1C) 6.24 0.16 0.16
 assign (segid 3A4 and resid 392 and name N) (segid HEM and resid 1 and name C1D) 4.22 0.08 0.08
 45 assign (segid 3A4 and resid 392 and name N) (segid HEM and resid 1 and name C2A) 6.45 0.05 0.06
 assign (segid 3A4 and resid 392 and name N) (segid HEM and resid 1 and name C2C) 6.71 0.15 0.14
 assign (segid 3A4 and resid 392 and name N) (segid HEM and resid 1 and name C2D) 4.36 0.12 0.13
 assign (segid 3A4 and resid 392 and name N) (segid HEM and resid 1 and name C3A) 7.09 0.11 0.11
 assign (segid 3A4 and resid 392 and name N) (segid HEM and resid 1 and name C3C) 6.14 0.15 0.15
 50 assign (segid 3A4 and resid 392 and name N) (segid HEM and resid 1 and name C3D) 4.33 0.12 0.12
 assign (segid 3A4 and resid 392 and name N) (segid HEM and resid 1 and name C4A) 6.52 0.13 0.13
 assign (segid 3A4 and resid 392 and name N) (segid HEM and resid 1 and name C4B) 7.11 0.16 0.17
 assign (segid 3A4 and resid 392 and name N) (segid HEM and resid 1 and name C4C) 5.22 0.16 0.16
 assign (segid 3A4 and resid 392 and name N) (segid HEM and resid 1 and name C4D) 4.21 0.06 0.06
 55 assign (segid 3A4 and resid 392 and name N) (segid HEM and resid 1 and name CAA) 7.12 0.09 0.10
 assign (segid 3A4 and resid 392 and name N) (segid HEM and resid 1 and name CAC) 6.68 0.14 0.15
 assign (segid 3A4 and resid 392 and name N) (segid HEM and resid 1 and name CAD) 5.01 0.15 0.15
 assign (segid 3A4 and resid 392 and name N) (segid HEM and resid 1 and name CBC) 7.40 0.29 0.30
 assign (segid 3A4 and resid 392 and name N) (segid HEM and resid 1 and name CBD) 4.41 0.17 0.17
 60 assign (segid 3A4 and resid 392 and name N) (segid HEM and resid 1 and name CGD) 5.69 0.19 0.19
 assign (segid 3A4 and resid 392 and name N) (segid HEM and resid 1 and name CHA) 4.82 0.08 0.07
 assign (segid 3A4 and resid 392 and name N) (segid HEM and resid 1 and name CHB) 7.27 0.17 0.18
 assign (segid 3A4 and resid 392 and name N) (segid HEM and resid 1 and name CHC) 7.01 0.16 0.16
 assign (segid 3A4 and resid 392 and name N) (segid HEM and resid 1 and name CHD) 4.78 0.10 0.10
 65 assign (segid 3A4 and resid 392 and name N) (segid HEM and resid 1 and name CMD) 5.14 0.17 0.17
 assign (segid 3A4 and resid 392 and name N) (segid HEM and resid 1 and name FE) 4.92 0.13 0.12
 assign (segid 3A4 and resid 392 and name N) (segid HEM and resid 1 and name NA) 5.45 0.09 0.09
 assign (segid 3A4 and resid 392 and name N) (segid HEM and resid 1 and name NB) 6.43 0.16 0.16
 assign (segid 3A4 and resid 392 and name N) (segid HEM and resid 1 and name NC) 5.30 0.17 0.17
 70 assign (segid 3A4 and resid 392 and name N) (segid HEM and resid 1 and name ND) 4.17 0.10 0.09
 assign (segid 3A4 and resid 392 and name N) (segid HEM and resid 1 and name O1D) 5.99 0.35 0.36
 assign (segid 3A4 and resid 392 and name N) (segid HEM and resid 1 and name O2D) 6.56 0.26 0.26
 assign (segid 3A4 and resid 392 and name O) (segid 3A4 and resid 392 and name CB) 3.24 0.09 0.09
 assign (segid 3A4 and resid 392 and name O) (segid 3A4 and resid 393 and name C) 3.44 0.08 0.08
 75 assign (segid 3A4 and resid 392 and name O) (segid 3A4 and resid 393 and name CA) 2.77 0.03 0.03
 assign (segid 3A4 and resid 392 and name O) (segid 3A4 and resid 393 and name N) 2.25 0.02 0.02
 assign (segid 3A4 and resid 392 and name O) (segid 3A4 and resid 393 and name O) 4.44 0.14 0.14
 assign (segid 3A4 and resid 392 and name O) (segid 3A4 and resid 394 and name C) 5.26 0.13 0.12
 assign (segid 3A4 and resid 392 and name O) (segid 3A4 and resid 394 and name CA) 4.73 0.10 0.10
 80 assign (segid 3A4 and resid 392 and name O) (segid 3A4 and resid 394 and name CB) 5.12 0.13 0.12
 assign (segid 3A4 and resid 392 and name O) (segid 3A4 and resid 394 and name N) 3.48 0.09 0.09
 assign (segid 3A4 and resid 392 and name O) (segid 3A4 and resid 394 and name O) 6.44 0.12 0.12
 assign (segid 3A4 and resid 392 and name O) (segid 3A4 and resid 395 and name C) 6.30 0.12 0.13
 assign (segid 3A4 and resid 392 and name O) (segid 3A4 and resid 395 and name CA) 5.72 0.15 0.15

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assign (segid 3A4 and resid 392 and name O ) (segid 3A4 and resid 395 and name N ) 4.72 0.13 0.14
assign (segid 3A4 and resid 392 and name O ) (segid 3A4 and resid 395 and name O ) 7.53 0.13 0.12
assign (segid 3A4 and resid 392 and name O ) (segid 3A4 and resid 396 and name C ) 7.47 0.14 0.13
assign (segid 3A4 and resid 392 and name O ) (segid 3A4 and resid 396 and name CA ) 6.62 0.17 0.18
5 assign (segid 3A4 and resid 392 and name O ) (segid 3A4 and resid 396 and name CB ) 6.21 0.26 0.25
assign (segid 3A4 and resid 392 and name O ) (segid 3A4 and resid 396 and name N ) 5.69 0.13 0.13
assign (segid 3A4 and resid 392 and name O ) (segid 3A4 and resid 397 and name CB ) 7.82 0.12 0.12
assign (segid 3A4 and resid 392 and name O ) (segid 3A4 and resid 397 and name N ) 7.07 0.10 0.10
assign (segid 3A4 and resid 392 and name O ) (segid HEM and resid 1 and name C1C) 6.85 0.22 0.23
10 assign (segid 3A4 and resid 392 and name O ) (segid HEM and resid 1 and name C1D) 6.30 0.19 0.20
assign (segid 3A4 and resid 392 and name O ) (segid HEM and resid 1 and name C2C) 6.71 0.28 0.27
assign (segid 3A4 and resid 392 and name O ) (segid HEM and resid 1 and name C2D) 6.69 0.21 0.21
assign (segid 3A4 and resid 392 and name O ) (segid HEM and resid 1 and name C3C) 6.25 0.29 0.30
assign (segid 3A4 and resid 392 and name O ) (segid HEM and resid 1 and name C3D) 7.22 0.17 0.17
15 assign (segid 3A4 and resid 392 and name O ) (segid HEM and resid 1 and name C4C) 6.12 0.26 0.26
assign (segid 3A4 and resid 392 and name O ) (segid HEM and resid 1 and name C4D) 7.24 0.12 0.11
assign (segid 3A4 and resid 392 and name O ) (segid HEM and resid 1 and name CAC) 6.37 0.31 0.32
assign (segid 3A4 and resid 392 and name O ) (segid HEM and resid 1 and name CBC) 6.54 0.49 0.49
assign (segid 3A4 and resid 392 and name O ) (segid HEM and resid 1 and name CBD) 7.49 0.14 0.15
20 assign (segid 3A4 and resid 392 and name O ) (segid HEM and resid 1 and name CHD) 6.08 0.23 0.23
assign (segid 3A4 and resid 392 and name O ) (segid HEM and resid 1 and name CMD) 6.93 0.25 0.26
assign (segid 3A4 and resid 392 and name O ) (segid HEM and resid 1 and name FE ) 7.05 0.18 0.17
assign (segid 3A4 and resid 392 and name O ) (segid HEM and resid 1 and name NC ) 6.49 0.21 0.22
assign (segid 3A4 and resid 392 and name O ) (segid HEM and resid 1 and name ND ) 6.70 0.15 0.14
25 assign (segid 3A4 and resid 393 and name C ) (segid 3A4 and resid 393 and name O ) 1.24 0.01 0.01
assign (segid 3A4 and resid 393 and name C ) (segid 3A4 and resid 394 and name C ) 3.01 0.09 0.09
assign (segid 3A4 and resid 393 and name C ) (segid 3A4 and resid 394 and name CA ) 2.45 0.02 0.02
assign (segid 3A4 and resid 393 and name C ) (segid 3A4 and resid 394 and name CB ) 3.71 0.02 0.02
30 assign (segid 3A4 and resid 393 and name C ) (segid 3A4 and resid 394 and name N ) 1.33 0.01 0.02
assign (segid 3A4 and resid 393 and name C ) (segid 3A4 and resid 394 and name O ) 3.88 0.13 0.12
assign (segid 3A4 and resid 393 and name C ) (segid 3A4 and resid 395 and name C ) 4.56 0.13 0.13
assign (segid 3A4 and resid 393 and name C ) (segid 3A4 and resid 395 and name CA ) 4.44 0.14 0.14
assign (segid 3A4 and resid 393 and name C ) (segid 3A4 and resid 395 and name N ) 3.24 0.10 0.11
35 assign (segid 3A4 and resid 393 and name C ) (segid 3A4 and resid 395 and name O ) 5.60 0.20 0.20
assign (segid 3A4 and resid 393 and name C ) (segid 3A4 and resid 396 and name C ) 4.83 0.06 0.07
assign (segid 3A4 and resid 393 and name C ) (segid 3A4 and resid 396 and name CA ) 4.61 0.07 0.07
assign (segid 3A4 and resid 393 and name C ) (segid 3A4 and resid 396 and name CB ) 4.50 0.20 0.20
40 assign (segid 3A4 and resid 393 and name C ) (segid 3A4 and resid 396 and name N ) 3.89 0.05 0.06
assign (segid 3A4 and resid 393 and name C ) (segid 3A4 and resid 396 and name O ) 6.04 0.07 0.07
assign (segid 3A4 and resid 393 and name C ) (segid 3A4 and resid 397 and name C ) 5.97 0.10 0.10
assign (segid 3A4 and resid 393 and name C ) (segid 3A4 and resid 397 and name CA ) 4.88 0.11 0.11
45 assign (segid 3A4 and resid 393 and name C ) (segid 3A4 and resid 397 and name CB ) 4.40 0.12 0.12
assign (segid 3A4 and resid 393 and name C ) (segid 3A4 and resid 397 and name N ) 4.04 0.08 0.09
assign (segid 3A4 and resid 393 and name C ) (segid 3A4 and resid 397 and name O ) 7.12 0.10 0.10
50 assign (segid 3A4 and resid 393 and name C ) (segid 3A4 and resid 398 and name CA ) 7.19 0.10 0.11
assign (segid 3A4 and resid 393 and name C ) (segid 3A4 and resid 398 and name CB ) 7.29 0.13 0.13
assign (segid 3A4 and resid 393 and name C ) (segid 3A4 and resid 398 and name CG ) 7.17 0.05 0.04
assign (segid 3A4 and resid 393 and name C ) (segid 3A4 and resid 398 and name N ) 5.89 0.11 0.11
55 assign (segid 3A4 and resid 393 and name C ) (segid 3A4 and resid 398 and name O ) 7.77 0.10 0.10
assign (segid 3A4 and resid 393 and name C ) (segid HEM and resid 1 and name C1B) 6.79 0.08 0.07
assign (segid 3A4 and resid 393 and name C ) (segid HEM and resid 1 and name C1C) 4.46 0.24 0.24
assign (segid 3A4 and resid 393 and name C ) (segid HEM and resid 1 and name C1D) 6.11 0.23 0.24
60 assign (segid 3A4 and resid 393 and name C ) (segid HEM and resid 1 and name C2B) 7.11 0.08 0.09
assign (segid 3A4 and resid 393 and name C ) (segid HEM and resid 1 and name C2C) 4.45 0.31 0.31
assign (segid 3A4 and resid 393 and name C ) (segid HEM and resid 1 and name C2D) 7.15 0.24 0.23
55 assign (segid 3A4 and resid 393 and name C ) (segid HEM and resid 1 and name C3B) 6.39 0.13 0.12
assign (segid 3A4 and resid 393 and name C ) (segid HEM and resid 1 and name C3C) 4.71 0.30 0.31
assign (segid 3A4 and resid 393 and name C ) (segid HEM and resid 1 and name C4A) 7.72 0.09 0.08
60 assign (segid 3A4 and resid 393 and name C ) (segid HEM and resid 1 and name C4B) 5.51 0.14 0.14
assign (segid 3A4 and resid 393 and name C ) (segid HEM and resid 1 and name C4C) 4.85 0.25 0.25
assign (segid 3A4 and resid 393 and name C ) (segid HEM and resid 1 and name C4D) 7.16 0.16 0.16
assign (segid 3A4 and resid 393 and name C ) (segid HEM and resid 1 and name CAB) 6.69 0.19 0.19
65 assign (segid 3A4 and resid 393 and name C ) (segid HEM and resid 1 and name CAC) 5.38 0.30 0.30
assign (segid 3A4 and resid 393 and name C ) (segid HEM and resid 1 and name CBC) 5.65 0.38 0.38
assign (segid 3A4 and resid 393 and name C ) (segid HEM and resid 1 and name CHB) 7.62 0.10 0.10
70 assign (segid 3A4 and resid 393 and name C ) (segid HEM and resid 1 and name CHC) 4.86 0.21 0.21
assign (segid 3A4 and resid 393 and name C ) (segid HEM and resid 1 and name CHD) 5.58 0.24 0.24
assign (segid 3A4 and resid 393 and name C ) (segid HEM and resid 1 and name CMC) 4.80 0.33 0.34
75 assign (segid 3A4 and resid 393 and name C ) (segid HEM and resid 1 and name FE ) 5.53 0.20 0.20
assign (segid 3A4 and resid 393 and name C ) (segid HEM and resid 1 and name NA ) 7.00 0.12 0.12
80 assign (segid 3A4 and resid 393 and name C ) (segid HEM and resid 1 and name NB ) 5.83 0.09 0.10
assign (segid 3A4 and resid 393 and name C ) (segid HEM and resid 1 and name NC ) 4.70 0.21 0.21
assign (segid 3A4 and resid 393 and name C ) (segid HEM and resid 1 and name ND ) 6.16 0.18 0.17
assign (segid 3A4 and resid 393 and name CA ) (segid 3A4 and resid 393 and name O ) 1.52 0.01 0.01
assign (segid 3A4 and resid 393 and name CA ) (segid 3A4 and resid 393 and name O ) 2.37 0.03 0.02
assign (segid 3A4 and resid 393 and name CA ) (segid 3A4 and resid 394 and name C ) 4.46 0.07 0.07
assign (segid 3A4 and resid 393 and name CA ) (segid 3A4 and resid 394 and name CA ) 3.83 0.03 0.03
assign (segid 3A4 and resid 393 and name CA ) (segid 3A4 and resid 394 and name CB ) 4.88 0.04 0.04
assign (segid 3A4 and resid 393 and name CA ) (segid 3A4 and resid 394 and name N ) 2.46 0.04 0.03
80 assign (segid 3A4 and resid 393 and name CA ) (segid 3A4 and resid 394 and name O ) 5.37 0.12 0.12
assign (segid 3A4 and resid 393 and name CA ) (segid 3A4 and resid 395 and name C ) 5.62 0.10 0.10
assign (segid 3A4 and resid 393 and name CA ) (segid 3A4 and resid 395 and name CA ) 5.56 0.10 0.11
assign (segid 3A4 and resid 393 and name CA ) (segid 3A4 and resid 395 and name N ) 4.46 0.06 0.07

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	assign (segid 3A4 and resid 393 and name N)	(segid HEM and resid 1 and name C4C)	3.99	0.24	0.25
	assign (segid 3A4 and resid 393 and name N)	(segid HEM and resid 1 and name C4D)	5.44	0.16	0.15
	assign (segid 3A4 and resid 393 and name N)	(segid HEM and resid 1 and name CAC)	4.78	0.25	0.24
	assign (segid 3A4 and resid 393 and name N)	(segid HEM and resid 1 and name CAD)	6.77	0.21	0.20
5	assign (segid 3A4 and resid 393 and name N)	(segid HEM and resid 1 and name CBC)	5.26	0.37	0.38
	assign (segid 3A4 and resid 393 and name N)	(segid HEM and resid 1 and name CBD)	6.57	0.18	0.19
	assign (segid 3A4 and resid 393 and name N)	(segid HEM and resid 1 and name CHA)	6.36	0.14	0.13
	assign (segid 3A4 and resid 393 and name N)	(segid HEM and resid 1 and name CHB)	7.64	0.13	0.13
	assign (segid 3A4 and resid 393 and name N)	(segid HEM and resid 1 and name CHC)	5.61	0.19	0.20
10	assign (segid 3A4 and resid 393 and name N)	(segid HEM and resid 1 and name CHD)	4.09	0.22	0.23
	assign (segid 3A4 and resid 393 and name N)	(segid HEM and resid 1 and name CMC)	5.70	0.22	0.22
	assign (segid 3A4 and resid 393 and name N)	(segid HEM and resid 1 and name CMD)	5.62	0.27	0.27
	assign (segid 3A4 and resid 393 and name N)	(segid HEM and resid 1 and name FE)	4.89	0.20	0.19
	assign (segid 3A4 and resid 393 and name N)	(segid HEM and resid 1 and name NA)	6.24	0.10	0.11
	assign (segid 3A4 and resid 393 and name N)	(segid HEM and resid 1 and name NB)	6.02	0.16	0.16
15	assign (segid 3A4 and resid 393 and name N)	(segid HEM and resid 1 and name NC)	4.27	0.22	0.22
	assign (segid 3A4 and resid 393 and name N)	(segid HEM and resid 1 and name ND)	4.67	0.17	0.18
	assign (segid 3A4 and resid 393 and name N)	(segid 3A4 and resid 394 and name C)	2.85	0.14	0.14
	assign (segid 3A4 and resid 393 and name O)	(segid 3A4 and resid 394 and name CA)	2.80	0.03	0.02
20	assign (segid 3A4 and resid 393 and name O)	(segid 3A4 and resid 394 and name CB)	4.25	0.03	0.04
	assign (segid 3A4 and resid 393 and name O)	(segid 3A4 and resid 394 and name N)	2.26	0.01	0.01
	assign (segid 3A4 and resid 393 and name O)	(segid 3A4 and resid 394 and name O)	3.40	0.17	0.18
	assign (segid 3A4 and resid 393 and name O)	(segid 3A4 and resid 395 and name C)	3.85	0.26	0.25
	assign (segid 3A4 and resid 393 and name O)	(segid 3A4 and resid 395 and name CA)	4.09	0.27	0.27
25	assign (segid 3A4 and resid 393 and name O)	(segid 3A4 and resid 395 and name N)	3.16	0.20	0.21
	assign (segid 3A4 and resid 393 and name O)	(segid 3A4 and resid 395 and name O)	4.77	0.29	0.30
	assign (segid 3A4 and resid 393 and name O)	(segid 3A4 and resid 396 and name C)	3.66	0.05	0.06
	assign (segid 3A4 and resid 393 and name O)	(segid 3A4 and resid 396 and name CA)	3.60	0.05	0.06
	assign (segid 3A4 and resid 393 and name O)	(segid 3A4 and resid 396 and name CB)	3.62	0.13	0.12
30	assign (segid 3A4 and resid 393 and name O)	(segid 3A4 and resid 396 and name N)	3.09	0.15	0.15
	assign (segid 3A4 and resid 393 and name O)	(segid 3A4 and resid 396 and name O)	4.85	0.06	0.07
	assign (segid 3A4 and resid 393 and name O)	(segid 3A4 and resid 397 and name C)	4.90	0.08	0.08
	assign (segid 3A4 and resid 393 and name O)	(segid 3A4 and resid 397 and name CA)	3.78	0.09	0.08
	assign (segid 3A4 and resid 393 and name O)	(segid 3A4 and resid 397 and name CB)	3.52	0.09	0.10
35	assign (segid 3A4 and resid 393 and name O)	(segid 3A4 and resid 397 and name N)	2.85	0.07	0.07
	assign (segid 3A4 and resid 393 and name O)	(segid 3A4 and resid 397 and name O)	6.03	0.07	0.08
	assign (segid 3A4 and resid 393 and name O)	(segid 3A4 and resid 398 and name C)	7.11	0.10	0.10
	assign (segid 3A4 and resid 393 and name O)	(segid 3A4 and resid 398 and name CA)	6.29	0.11	0.11
	assign (segid 3A4 and resid 393 and name O)	(segid 3A4 and resid 398 and name CB)	6.55	0.16	0.17
40	assign (segid 3A4 and resid 393 and name O)	(segid 3A4 and resid 398 and name CD1)	7.19	0.28	0.27
	assign (segid 3A4 and resid 393 and name O)	(segid 3A4 and resid 398 and name CG)	6.61	0.08	0.08
	assign (segid 3A4 and resid 393 and name O)	(segid 3A4 and resid 398 and name N)	4.93	0.11	0.10
	assign (segid 3A4 and resid 393 and name O)	(segid 3A4 and resid 399 and name N)	6.73	0.14	0.14
	assign (segid 3A4 and resid 393 and name O)	(segid 3A4 and resid 400 and name N)	7.71	0.08	0.08
45	assign (segid 3A4 and resid 393 and name O)	(segid HEM and resid 1 and name C1B)	7.06	0.16	0.16
	assign (segid 3A4 and resid 393 and name O)	(segid HEM and resid 1 and name C1C)	4.50	0.28	0.29
	assign (segid 3A4 and resid 393 and name O)	(segid HEM and resid 1 and name C1D)	6.90	0.27	0.26
	assign (segid 3A4 and resid 393 and name O)	(segid HEM and resid 1 and name C2B)	7.16	0.18	0.17
	assign (segid 3A4 and resid 393 and name O)	(segid HEM and resid 1 and name C2C)	4.32	0.35	0.35
50	assign (segid 3A4 and resid 393 and name O)	(segid HEM and resid 1 and name C3B)	6.26	0.20	0.19
	assign (segid 3A4 and resid 393 and name O)	(segid HEM and resid 1 and name C3C)	4.85	0.33	0.32
	assign (segid 3A4 and resid 393 and name O)	(segid HEM and resid 1 and name C4B)	5.53	0.21	0.22
	assign (segid 3A4 and resid 393 and name O)	(segid HEM and resid 1 and name C4C)	5.27	0.26	0.25
	assign (segid 3A4 and resid 393 and name O)	(segid HEM and resid 1 and name CAB)	6.31	0.27	0.27
55	assign (segid 3A4 and resid 393 and name O)	(segid HEM and resid 1 and name CAC)	5.48	0.32	0.32
	assign (segid 3A4 and resid 393 and name O)	(segid HEM and resid 1 and name CBC)	5.59	0.35	0.36
	assign (segid 3A4 and resid 393 and name O)	(segid HEM and resid 1 and name CHC)	4.74	0.27	0.27
	assign (segid 3A4 and resid 393 and name O)	(segid HEM and resid 1 and name CHD)	6.20	0.27	0.26
	assign (segid 3A4 and resid 393 and name O)	(segid HEM and resid 1 and name CMC)	4.28	0.41	0.41
60	assign (segid 3A4 and resid 393 and name O)	(segid HEM and resid 1 and name FE)	6.13	0.28	0.28
	assign (segid 3A4 and resid 393 and name O)	(segid HEM and resid 1 and name NB)	6.12	0.17	0.17
	assign (segid 3A4 and resid 393 and name O)	(segid HEM and resid 1 and name NC)	5.08	0.24	0.23
	assign (segid 3A4 and resid 393 and name O)	(segid HEM and resid 1 and name ND)	6.96	0.22	0.22
	assign (segid 3A4 and resid 394 and name C)	(segid 3A4 and resid 394 and name CB)	2.48	0.03	0.02
65	assign (segid 3A4 and resid 394 and name C)	(segid 3A4 and resid 395 and name C)	1.24	0.01	0.00
	assign (segid 3A4 and resid 394 and name C)	(segid 3A4 and resid 395 and name CA)	3.06	0.07	0.07
	assign (segid 3A4 and resid 394 and name C)	(segid 3A4 and resid 395 and name N)	2.44	0.01	0.02
	assign (segid 3A4 and resid 394 and name C)	(segid 3A4 and resid 395 and name O)	1.33	0.02	0.01
	assign (segid 3A4 and resid 394 and name C)	(segid 3A4 and resid 395 and name O)	3.84	0.18	0.19
70	assign (segid 3A4 and resid 394 and name C)	(segid 3A4 and resid 396 and name C)	4.56	0.05	0.05
	assign (segid 3A4 and resid 394 and name C)	(segid 3A4 and resid 396 and name CA)	4.54	0.05	0.05
	assign (segid 3A4 and resid 394 and name C)	(segid 3A4 and resid 396 and name CB)	5.36	0.11	0.11
	assign (segid 3A4 and resid 394 and name C)	(segid 3A4 and resid 396 and name N)	3.39	0.06	0.05
	assign (segid 3A4 and resid 394 and name C)	(segid 3A4 and resid 396 and name O)	5.59	0.06	0.07
75	assign (segid 3A4 and resid 394 and name C)	(segid 3A4 and resid 397 and name C)	4.82	0.09	0.10
	assign (segid 3A4 and resid 394 and name C)	(segid 3A4 and resid 397 and name CA)	4.51	0.09	0.09
	assign (segid 3A4 and resid 394 and name C)	(segid 3A4 and resid 397 and name CB)	4.23	0.12	0.12
	assign (segid 3A4 and resid 394 and name C)	(segid 3A4 and resid 397 and name N)	3.83	0.08	0.08
	assign (segid 3A4 and resid 394 and name C)	(segid 3A4 and resid 397 and name O)	6.04	0.08	0.09
80	assign (segid 3A4 and resid 394 and name C)	(segid 3A4 and resid 398 and name C)	6.08	0.03	0.03
	assign (segid 3A4 and resid 394 and name C)	(segid 3A4 and resid 398 and name CA)	5.04	0.06	0.07
	assign (segid 3A4 and resid 394 and name C)	(segid 3A4 and resid 398 and name CB)	4.68	0.06	0.06
	assign (segid 3A4 and resid 394 and name C)	(segid 3A4 and resid 398 and name CD1)	4.67	0.23	0.23

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	assign (segid 3A4 and resid 394 and name CB)	(segid 3A4 and resid 395 and name O)	6.24	0.20	0.20
	assign (segid 3A4 and resid 394 and name CB)	(segid 3A4 and resid 396 and name C)	6.89	0.06	0.07
	assign (segid 3A4 and resid 394 and name CB)	(segid 3A4 and resid 396 and name CA)	6.86	0.05	0.06
	assign (segid 3A4 and resid 394 and name CB)	(segid 3A4 and resid 396 and name CB)	7.43	0.16	0.16
5	assign (segid 3A4 and resid 394 and name CB)	(segid 3A4 and resid 396 and name N)	5.69	0.06	0.06
	assign (segid 3A4 and resid 394 and name CB)	(segid 3A4 and resid 397 and name C)	6.80	0.16	0.16
	assign (segid 3A4 and resid 394 and name CB)	(segid 3A4 and resid 397 and name CA)	6.42	0.16	0.15
	assign (segid 3A4 and resid 394 and name CB)	(segid 3A4 and resid 397 and name CB)	5.64	0.20	0.20
	assign (segid 3A4 and resid 394 and name CB)	(segid 3A4 and resid 397 and name N)	5.99	0.10	0.09
10	assign (segid 3A4 and resid 394 and name CB)	(segid 3A4 and resid 398 and name CA)	6.91	0.12	0.12
	assign (segid 3A4 and resid 394 and name CB)	(segid 3A4 and resid 398 and name CB)	6.33	0.08	0.07
	assign (segid 3A4 and resid 394 and name CB)	(segid 3A4 and resid 398 and name CD1)	5.38	0.24	0.23
	assign (segid 3A4 and resid 394 and name CB)	(segid 3A4 and resid 398 and name CG)	5.58	0.11	0.12
	assign (segid 3A4 and resid 394 and name CB)	(segid 3A4 and resid 398 and name N)	6.12	0.13	0.14
	assign (segid 3A4 and resid 394 and name CB)	(segid 3A4 and resid 399 and name CA)	9.56	0.06	0.06
15	assign (segid 3A4 and resid 394 and name CB)	(segid 3A4 and resid 399 and name CB)	9.66	0.12	0.11
	assign (segid 3A4 and resid 394 and name CB)	(segid 3A4 and resid 399 and name CB)	11.25	0.09	0.09
	assign (segid 3A4 and resid 394 and name CB)	(segid 3A4 and resid 400 and name CA)	10.96	0.10	0.11
	assign (segid 3A4 and resid 394 and name CB)	(segid 3A4 and resid 400 and name CB)	11.56	0.15	0.15
	assign (segid 3A4 and resid 394 and name CB)	(segid 3A4 and resid 401 and name CA)	12.93	0.11	0.11
20	assign (segid 3A4 and resid 394 and name CB)	(segid 3A4 and resid 402 and name CA)	12.35	0.13	0.13
	assign (segid 3A4 and resid 394 and name CB)	(segid 3A4 and resid 402 and name CB)	15.16	0.04	0.04
	assign (segid 3A4 and resid 394 and name CB)	(segid 3A4 and resid 403 and name CB)	14.92	0.03	0.02
	assign (segid 3A4 and resid 394 and name CB)	(segid 3A4 and resid 404 and name CA)	16.46	0.12	0.12
	assign (segid 3A4 and resid 394 and name CB)	(segid 3A4 and resid 404 and name CB)	15.84	0.13	0.14
25	assign (segid 3A4 and resid 394 and name CB)	(segid 3A4 and resid 405 and name CA)	17.27	0.04	0.04
	assign (segid 3A4 and resid 394 and name CB)	(segid 3A4 and resid 405 and name CB)	16.46	0.07	0.08
	assign (segid 3A4 and resid 394 and name CB)	(segid 3A4 and resid 406 and name CA)	18.83	0.07	0.08
	assign (segid 3A4 and resid 394 and name CB)	(segid 3A4 and resid 433 and name CA)	18.11	0.37	0.36
30	assign (segid 3A4 and resid 394 and name CB)	(segid HEM and resid 1 and name C1B)	7.01	0.18	0.19
	assign (segid 3A4 and resid 394 and name CB)	(segid HEM and resid 1 and name C1C)	6.93	0.24	0.24
	assign (segid 3A4 and resid 394 and name CB)	(segid HEM and resid 1 and name C2B)	7.22	0.20	0.21
	assign (segid 3A4 and resid 394 and name CB)	(segid HEM and resid 1 and name C3B)	7.04	0.22	0.21
	assign (segid 3A4 and resid 394 and name CB)	(segid HEM and resid 1 and name C4A)	7.59	0.16	0.17
35	assign (segid 3A4 and resid 394 and name CB)	(segid HEM and resid 1 and name C4B)	6.70	0.21	0.22
	assign (segid 3A4 and resid 394 and name CB)	(segid HEM and resid 1 and name CHB)	7.43	0.20	0.20
	assign (segid 3A4 and resid 394 and name CB)	(segid HEM and resid 1 and name CHC)	6.79	0.25	0.25
	assign (segid 3A4 and resid 394 and name CB)	(segid HEM and resid 1 and name FE)	6.77	0.19	0.19
	assign (segid 3A4 and resid 394 and name CB)	(segid HEM and resid 1 and name NA)	7.35	0.13	0.13
40	assign (segid 3A4 and resid 394 and name CB)	(segid HEM and resid 1 and name NB)	6.71	0.16	0.16
	assign (segid 3A4 and resid 394 and name CB)	(segid HEM and resid 1 and name NC)	6.98	0.18	0.18
	assign (segid 3A4 and resid 394 and name CB)	(segid HEM and resid 1 and name ND)	7.68	0.09	0.08
	assign (segid 3A4 and resid 394 and name CB)	(segid 3A4 and resid 394 and name C)	2.50	0.02	0.03
	assign (segid 3A4 and resid 394 and name N)	(segid 3A4 and resid 394 and name CA)	1.46	0.00	0.01
45	assign (segid 3A4 and resid 394 and name N)	(segid 3A4 and resid 394 and name CB)	2.46	0.02	0.02
	assign (segid 3A4 and resid 394 and name N)	(segid 3A4 and resid 394 and name O)	3.53	0.05	0.05
	assign (segid 3A4 and resid 394 and name N)	(segid 3A4 and resid 395 and name C)	4.82	0.06	0.06
	assign (segid 3A4 and resid 394 and name N)	(segid 3A4 and resid 395 and name CA)	4.32	0.05	0.04
	assign (segid 3A4 and resid 394 and name N)	(segid 3A4 and resid 395 and name N)	2.90	0.03	0.04
50	assign (segid 3A4 and resid 394 and name N)	(segid 3A4 and resid 395 and name O)	5.85	0.15	0.15
	assign (segid 3A4 and resid 394 and name N)	(segid 3A4 and resid 396 and name C)	5.63	0.05	0.06
	assign (segid 3A4 and resid 394 and name N)	(segid 3A4 and resid 396 and name CA)	5.46	0.12	0.11
	assign (segid 3A4 and resid 394 and name N)	(segid 3A4 and resid 396 and name CB)	5.60	0.24	0.24
	assign (segid 3A4 and resid 394 and name N)	(segid 3A4 and resid 396 and name N)	4.49	0.10	0.10
55	assign (segid 3A4 and resid 394 and name N)	(segid 3A4 and resid 396 and name O)	6.82	0.05	0.05
	assign (segid 3A4 and resid 394 and name N)	(segid 3A4 and resid 397 and name C)	6.33	0.11	0.10
	assign (segid 3A4 and resid 394 and name N)	(segid 3A4 and resid 397 and name CA)	5.46	0.12	0.12
	assign (segid 3A4 and resid 394 and name N)	(segid 3A4 and resid 397 and name CB)	4.79	0.16	0.16
	assign (segid 3A4 and resid 394 and name N)	(segid 3A4 and resid 397 and name N)	4.76	0.07	0.07
60	assign (segid 3A4 and resid 394 and name N)	(segid 3A4 and resid 397 and name O)	7.51	0.10	0.11
	assign (segid 3A4 and resid 394 and name N)	(segid 3A4 and resid 398 and name CA)	7.20	0.09	0.08
	assign (segid 3A4 and resid 394 and name N)	(segid 3A4 and resid 398 and name CB)	7.05	0.08	0.09
	assign (segid 3A4 and resid 394 and name N)	(segid 3A4 and resid 398 and name CD1)	6.91	0.24	0.24
	assign (segid 3A4 and resid 394 and name N)	(segid 3A4 and resid 398 and name CG)	6.71	0.04	0.03
65	assign (segid 3A4 and resid 394 and name N)	(segid 3A4 and resid 398 and name N)	6.03	0.10	0.09
	assign (segid 3A4 and resid 394 and name N)	(segid HEM and resid 1 and name C1A)	7.48	0.09	0.08
	assign (segid 3A4 and resid 394 and name N)	(segid HEM and resid 1 and name C1B)	6.59	0.17	0.17
	assign (segid 3A4 and resid 394 and name N)	(segid HEM and resid 1 and name C1C)	5.12	0.26	0.25
	assign (segid 3A4 and resid 394 and name N)	(segid HEM and resid 1 and name C1D)	6.43	0.19	0.18
70	assign (segid 3A4 and resid 394 and name N)	(segid HEM and resid 1 and name C2B)	6.95	0.15	0.16
	assign (segid 3A4 and resid 394 and name N)	(segid HEM and resid 1 and name C2C)	5.42	0.30	0.29
	assign (segid 3A4 and resid 394 and name N)	(segid HEM and resid 1 and name C2D)	7.39	0.18	0.19
	assign (segid 3A4 and resid 394 and name N)	(segid HEM and resid 1 and name C3B)	6.43	0.17	0.18
	assign (segid 3A4 and resid 394 and name N)	(segid HEM and resid 1 and name C3C)	5.68	0.28	0.29
	assign (segid 3A4 and resid 394 and name N)	(segid HEM and resid 1 and name C4A)	7.32	0.14	0.14
75	assign (segid 3A4 and resid 394 and name N)	(segid HEM and resid 1 and name C4B)	5.69	0.19	0.19
	assign (segid 3A4 and resid 394 and name N)	(segid HEM and resid 1 and name C4C)	5.55	0.25	0.24
	assign (segid 3A4 and resid 394 and name N)	(segid HEM and resid 1 and name C4D)	7.08	0.11	0.12
	assign (segid 3A4 and resid 394 and name N)	(segid HEM and resid 1 and name CAB)	6.86	0.21	0.21
80	assign (segid 3A4 and resid 394 and name N)	(segid HEM and resid 1 and name CAC)	6.47	0.28	0.28
	assign (segid 3A4 and resid 394 and name N)	(segid HEM and resid 1 and name CBC)	6.85	0.37	0.37
	assign (segid 3A4 and resid 394 and name N)	(segid HEM and resid 1 and name CHA)	7.62	0.08	0.09
	assign (segid 3A4 and resid 394 and name N)	(segid HEM and resid 1 and name CHB)	7.25	0.20	0.20

	assign (segid 3A4 and resid 394 and name N)	(segid HEM and resid 1 and name CHC)	5.34	0.24	0.24
	assign (segid 3A4 and resid 394 and name N)	(segid HEM and resid 1 and name CHD)	6.16	0.20	0.20
	assign (segid 3A4 and resid 394 and name N)	(segid HEM and resid 1 and name CMC)	5.90	0.32	0.31
	assign (segid 3A4 and resid 394 and name N)	(segid HEM and resid 1 and name FE)	5.56	0.15	0.15
5	assign (segid 3A4 and resid 394 and name N)	(segid HEM and resid 1 and name NA)	6.72	0.10	0.09
	assign (segid 3A4 and resid 394 and name N)	(segid HEM and resid 1 and name NB)	5.83	0.18	0.17
	assign (segid 3A4 and resid 394 and name N)	(segid HEM and resid 1 and name NC)	5.19	0.22	0.23
	assign (segid 3A4 and resid 394 and name N)	(segid HEM and resid 1 and name ND)	6.25	0.13	0.14
	assign (segid 3A4 and resid 394 and name O)	(segid 3A4 and resid 394 and name CB)	3.26	0.08	0.07
10	assign (segid 3A4 and resid 394 and name O)	(segid 3A4 and resid 395 and name C)	3.04	0.14	0.14
	assign (segid 3A4 and resid 394 and name O)	(segid 3A4 and resid 395 and name CA)	2.77	0.03	0.04
	assign (segid 3A4 and resid 394 and name O)	(segid 3A4 and resid 395 and name N)	2.24	0.02	0.03
	assign (segid 3A4 and resid 394 and name O)	(segid 3A4 and resid 395 and name O)	3.44	0.27	0.28
	assign (segid 3A4 and resid 394 and name O)	(segid 3A4 and resid 396 and name C)	4.20	0.09	0.09
15	assign (segid 3A4 and resid 394 and name O)	(segid 3A4 and resid 396 and name CA)	4.52	0.11	0.10
	assign (segid 3A4 and resid 394 and name O)	(segid 3A4 and resid 396 and name CB)	5.56	0.06	0.06
	assign (segid 3A4 and resid 394 and name O)	(segid 3A4 and resid 396 and name N)	3.58	0.07	0.08
	assign (segid 3A4 and resid 394 and name O)	(segid 3A4 and resid 396 and name O)	5.05	0.05	0.06
	assign (segid 3A4 and resid 394 and name O)	(segid 3A4 and resid 397 and name C)	3.85	0.09	0.08
20	assign (segid 3A4 and resid 394 and name O)	(segid 3A4 and resid 397 and name CA)	3.83	0.11	0.12
	assign (segid 3A4 and resid 394 and name O)	(segid 3A4 and resid 397 and name CB)	3.66	0.11	0.12
	assign (segid 3A4 and resid 394 and name O)	(segid 3A4 and resid 397 and name N)	3.43	0.14	0.14
	assign (segid 3A4 and resid 394 and name O)	(segid 3A4 and resid 397 and name O)	5.02	0.08	0.09
	assign (segid 3A4 and resid 394 and name O)	(segid 3A4 and resid 398 and name C)	4.98	0.04	0.04
25	assign (segid 3A4 and resid 394 and name O)	(segid 3A4 and resid 398 and name CA)	3.85	0.06	0.07
	assign (segid 3A4 and resid 394 and name O)	(segid 3A4 and resid 398 and name CB)	3.54	0.06	0.05
	assign (segid 3A4 and resid 394 and name O)	(segid 3A4 and resid 398 and name CD1)	3.81	0.18	0.19
	assign (segid 3A4 and resid 394 and name O)	(segid 3A4 and resid 398 and name CG)	3.39	0.10	0.10
	assign (segid 3A4 and resid 394 and name O)	(segid 3A4 and resid 398 and name N)	3.00	0.09	0.08
30	assign (segid 3A4 and resid 394 and name O)	(segid 3A4 and resid 398 and name O)	6.11	0.04	0.04
	assign (segid 3A4 and resid 394 and name O)	(segid 3A4 and resid 399 and name C)	7.25	0.07	0.06
	assign (segid 3A4 and resid 394 and name O)	(segid 3A4 and resid 399 and name CA)	6.36	0.07	0.07
	assign (segid 3A4 and resid 394 and name O)	(segid 3A4 and resid 399 and name CB)	6.59	0.12	0.11
	assign (segid 3A4 and resid 394 and name O)	(segid 3A4 and resid 399 and name N)	5.00	0.06	0.06
35	assign (segid 3A4 and resid 394 and name O)	(segid 3A4 and resid 400 and name N)	7.03	0.07	0.07
	assign (segid 3A4 and resid 394 and name O)	(segid 3A4 and resid 401 and name N)	7.84	0.05	0.05
	assign (segid 3A4 and resid 394 and name O)	(segid HEM and resid 1 and name C1C)	7.01	0.23	0.23
	assign (segid 3A4 and resid 394 and name O)	(segid HEM and resid 1 and name C2B)	7.64	0.15	0.15
	assign (segid 3A4 and resid 394 and name O)	(segid HEM and resid 1 and name C2C)	7.22	0.29	0.29
40	assign (segid 3A4 and resid 394 and name O)	(segid HEM and resid 1 and name C3B)	6.99	0.15	0.15
	assign (segid 3A4 and resid 394 and name O)	(segid HEM and resid 1 and name C4B)	6.91	0.16	0.16
	assign (segid 3A4 and resid 394 and name O)	(segid HEM and resid 1 and name CAB)	6.78	0.20	0.19
	assign (segid 3A4 and resid 394 and name O)	(segid HEM and resid 1 and name CBB)	7.11	0.23	0.23
	assign (segid 3A4 and resid 394 and name O)	(segid HEM and resid 1 and name CHC)	6.64	0.22	0.22
45	assign (segid 3A4 and resid 394 and name O)	(segid HEM and resid 1 and name CMC)	7.00	0.35	0.36
	assign (segid 3A4 and resid 394 and name O)	(segid HEM and resid 1 and name NB)	7.52	0.16	0.17
	assign (segid 3A4 and resid 395 and name C)	(segid 3A4 and resid 395 and name O)	1.24	0.01	0.01
	assign (segid 3A4 and resid 395 and name C)	(segid 3A4 and resid 396 and name C)	3.04	0.03	0.03
	assign (segid 3A4 and resid 395 and name C)	(segid 3A4 and resid 396 and name CA)	2.44	0.01	0.01
50	assign (segid 3A4 and resid 395 and name C)	(segid 3A4 and resid 396 and name CB)	3.73	0.02	0.02
	assign (segid 3A4 and resid 395 and name C)	(segid 3A4 and resid 396 and name N)	1.33	0.01	0.01
	assign (segid 3A4 and resid 395 and name C)	(segid 3A4 and resid 396 and name O)	3.85	0.10	0.10
	assign (segid 3A4 and resid 395 and name C)	(segid 3A4 and resid 397 and name C)	4.60	0.07	0.06
	assign (segid 3A4 and resid 395 and name C)	(segid 3A4 and resid 397 and name CA)	4.50	0.06	0.07
55	assign (segid 3A4 and resid 395 and name C)	(segid 3A4 and resid 397 and name CB)	5.20	0.09	0.09
	assign (segid 3A4 and resid 395 and name C)	(segid 3A4 and resid 397 and name N)	3.32	0.08	0.09
	assign (segid 3A4 and resid 395 and name C)	(segid 3A4 and resid 397 and name O)	5.66	0.08	0.08
	assign (segid 3A4 and resid 395 and name C)	(segid 3A4 and resid 398 and name C)	4.96	0.05	0.06
	assign (segid 3A4 and resid 395 and name C)	(segid 3A4 and resid 398 and name CA)	4.70	0.06	0.05
60	assign (segid 3A4 and resid 395 and name C)	(segid 3A4 and resid 398 and name CB)	4.61	0.10	0.10
	assign (segid 3A4 and resid 395 and name C)	(segid 3A4 and resid 398 and name CD1)	5.70	0.20	0.21
	assign (segid 3A4 and resid 395 and name C)	(segid 3A4 and resid 398 and name CG)	5.37	0.07	0.07
	assign (segid 3A4 and resid 395 and name C)	(segid 3A4 and resid 398 and name N)	3.92	0.06	0.06
	assign (segid 3A4 and resid 395 and name C)	(segid 3A4 and resid 398 and name O)	6.16	0.06	0.06
65	assign (segid 3A4 and resid 395 and name C)	(segid 3A4 and resid 399 and name C)	6.14	0.14	0.14
	assign (segid 3A4 and resid 395 and name C)	(segid 3A4 and resid 399 and name CA)	5.06	0.14	0.14
	assign (segid 3A4 and resid 395 and name C)	(segid 3A4 and resid 399 and name CB)	4.61	0.21	0.20
	assign (segid 3A4 and resid 395 and name C)	(segid 3A4 and resid 399 and name N)	4.20	0.10	0.10
	assign (segid 3A4 and resid 395 and name C)	(segid 3A4 and resid 399 and name O)	7.30	0.12	0.12
70	assign (segid 3A4 and resid 395 and name C)	(segid 3A4 and resid 400 and name CA)	7.32	0.13	0.13
	assign (segid 3A4 and resid 395 and name C)	(segid 3A4 and resid 400 and name CB)	7.33	0.17	0.17
	assign (segid 3A4 and resid 395 and name C)	(segid 3A4 and resid 400 and name N)	6.04	0.14	0.14
	assign (segid 3A4 and resid 395 and name CA)	(segid 3A4 and resid 395 and name C)	1.52	0.00	0.01
	assign (segid 3A4 and resid 395 and name CA)	(segid 3A4 and resid 395 and name O)	2.39	0.01	0.01
75	assign (segid 3A4 and resid 395 and name CA)	(segid 3A4 and resid 396 and name C)	4.41	0.05	0.04
	assign (segid 3A4 and resid 395 and name CA)	(segid 3A4 and resid 396 and name CA)	3.81	0.02	0.01
	assign (segid 3A4 and resid 395 and name CA)	(segid 3A4 and resid 396 and name CB)	4.87	0.02	0.02
	assign (segid 3A4 and resid 395 and name CA)	(segid 3A4 and resid 396 and name N)	2.43	0.01	0.01
	assign (segid 3A4 and resid 395 and name CA)	(segid 3A4 and resid 396 and name O)	5.29	0.11	0.12
80	assign (segid 3A4 and resid 395 and name CA)	(segid 3A4 and resid 397 and name C)	5.52	0.09	0.09
	assign (segid 3A4 and resid 395 and name CA)	(segid 3A4 and resid 397 and name CA)	5.45	0.04	0.04
	assign (segid 3A4 and resid 395 and name CA)	(segid 3A4 and resid 397 and name CB)	5.81	0.07	0.06
	assign (segid 3A4 and resid 395 and name CA)	(segid 3A4 and resid 397 and name N)	4.38	0.05	0.06

	assign (segid 3A4 and resid 395 and name CA)	(segid 3A4 and resid 397 and name O)	6.66	0.11	0.10
	assign (segid 3A4 and resid 395 and name CA)	(segid 3A4 and resid 398 and name C)	5.80	0.13	0.13
	assign (segid 3A4 and resid 395 and name CA)	(segid 3A4 and resid 398 and name CA)	5.28	0.09	0.09
	assign (segid 3A4 and resid 395 and name CA)	(segid 3A4 and resid 398 and name CB)	4.79	0.07	0.08
5	assign (segid 3A4 and resid 395 and name CA)	(segid 3A4 and resid 398 and name CD1)	5.19	0.19	0.19
	assign (segid 3A4 and resid 395 and name CA)	(segid 3A4 and resid 398 and name CG)	5.23	0.08	0.08
	assign (segid 3A4 and resid 395 and name CA)	(segid 3A4 and resid 398 and name N)	4.64	0.09	0.09
	assign (segid 3A4 and resid 395 and name CA)	(segid 3A4 and resid 398 and name O)	6.97	0.13	0.13
	assign (segid 3A4 and resid 395 and name CA)	(segid 3A4 and resid 399 and name C)	7.41	0.18	0.17
10	assign (segid 3A4 and resid 395 and name CA)	(segid 3A4 and resid 399 and name CA)	11.70	0.19	0.19
	assign (segid 3A4 and resid 395 and name CA)	(segid 3A4 and resid 399 and name CB)	5.85	0.24	0.24
	assign (segid 3A4 and resid 395 and name CA)	(segid 3A4 and resid 399 and name N)	5.25	0.17	0.17
	assign (segid 3A4 and resid 395 and name CA)	(segid 3A4 and resid 400 and name CA)	8.70	0.15	0.16
	assign (segid 3A4 and resid 395 and name CA)	(segid 3A4 and resid 400 and name CB)	8.74	0.18	0.18
	assign (segid 3A4 and resid 395 and name CA)	(segid 3A4 and resid 400 and name N)	7.40	0.17	0.17
15	assign (segid 3A4 and resid 395 and name CA)	(segid 3A4 and resid 401 and name CA)	10.04	0.14	0.13
	assign (segid 3A4 and resid 395 and name CA)	(segid 3A4 and resid 402 and name CA)	10.66	0.22	0.22
	assign (segid 3A4 and resid 395 and name CA)	(segid 3A4 and resid 402 and name CB)	9.87	0.27	0.26
	assign (segid 3A4 and resid 395 and name CA)	(segid 3A4 and resid 403 and name CA)	12.19	0.10	0.10
20	assign (segid 3A4 and resid 395 and name CA)	(segid 3A4 and resid 403 and name CB)	11.70	0.10	0.09
	assign (segid 3A4 and resid 395 and name CA)	(segid 3A4 and resid 404 and name CA)	14.20	0.06	0.06
	assign (segid 3A4 and resid 395 and name CA)	(segid 3A4 and resid 404 and name CB)	13.88	0.10	0.10
	assign (segid 3A4 and resid 395 and name CA)	(segid 3A4 and resid 405 and name CA)	15.50	0.16	0.17
	assign (segid 3A4 and resid 395 and name CA)	(segid 3A4 and resid 405 and name CB)	14.96	0.17	0.16
25	assign (segid 3A4 and resid 395 and name CA)	(segid 3A4 and resid 406 and name CA)	16.40	0.17	0.17
	assign (segid 3A4 and resid 395 and name CA)	(segid 3A4 and resid 407 and name CA)	18.25	0.05	0.05
	assign (segid 3A4 and resid 395 and name CA)	(segid 3A4 and resid 407 and name CB)	17.77	0.10	0.10
	assign (segid 3A4 and resid 395 and name N)	(segid 3A4 and resid 395 and name C)	2.45	0.01	0.02
30	assign (segid 3A4 and resid 395 and name N)	(segid 3A4 and resid 395 and name CA)	1.46	0.01	0.01
	assign (segid 3A4 and resid 395 and name N)	(segid 3A4 and resid 395 and name O)	3.46	0.07	0.08
	assign (segid 3A4 and resid 395 and name N)	(segid 3A4 and resid 396 and name C)	4.66	0.10	0.09
	assign (segid 3A4 and resid 395 and name N)	(segid 3A4 and resid 396 and name CA)	4.21	0.09	0.09
	assign (segid 3A4 and resid 395 and name N)	(segid 3A4 and resid 396 and name CB)	5.00	0.14	0.13
35	assign (segid 3A4 and resid 395 and name N)	(segid 3A4 and resid 396 and name N)	2.83	0.09	0.09
	assign (segid 3A4 and resid 395 and name N)	(segid 3A4 and resid 396 and name O)	5.72	0.14	0.13
	assign (segid 3A4 and resid 395 and name N)	(segid 3A4 and resid 397 and name C)	5.57	0.11	0.10
	assign (segid 3A4 and resid 395 and name N)	(segid 3A4 and resid 397 and name CA)	5.24	0.08	0.08
	assign (segid 3A4 and resid 395 and name N)	(segid 3A4 and resid 397 and name CB)	5.24	0.10	0.09
40	assign (segid 3A4 and resid 395 and name N)	(segid 3A4 and resid 397 and name N)	4.26	0.07	0.06
	assign (segid 3A4 and resid 395 and name N)	(segid 3A4 and resid 398 and name C)	6.78	0.10	0.10
	assign (segid 3A4 and resid 395 and name N)	(segid 3A4 and resid 398 and name CA)	6.47	0.08	0.09
	assign (segid 3A4 and resid 395 and name N)	(segid 3A4 and resid 398 and name CB)	5.67	0.07	0.06
	assign (segid 3A4 and resid 395 and name N)	(segid 3A4 and resid 398 and name CD1)	5.23	0.05	0.05
45	assign (segid 3A4 and resid 395 and name N)	(segid 3A4 and resid 398 and name CG)	5.28	0.20	0.21
	assign (segid 3A4 and resid 395 and name N)	(segid 3A4 and resid 398 and name N)	5.30	0.05	0.05
	assign (segid 3A4 and resid 395 and name N)	(segid 3A4 and resid 398 and name O)	4.81	0.08	0.09
	assign (segid 3A4 and resid 395 and name N)	(segid 3A4 and resid 399 and name C)	7.66	0.07	0.08
	assign (segid 3A4 and resid 395 and name N)	(segid 3A4 and resid 399 and name CA)	7.21	0.14	0.15
50	assign (segid 3A4 and resid 395 and name N)	(segid 3A4 and resid 399 and name CB)	6.98	0.21	0.20
	assign (segid 3A4 and resid 395 and name O)	(segid 3A4 and resid 396 and name C)	6.10	0.12	0.12
	assign (segid 3A4 and resid 395 and name O)	(segid 3A4 and resid 396 and name CA)	3.03	0.05	0.06
	assign (segid 3A4 and resid 395 and name O)	(segid 3A4 and resid 396 and name CB)	2.79	0.03	0.04
	assign (segid 3A4 and resid 395 and name O)	(segid 3A4 and resid 396 and name N)	4.29	0.03	0.03
55	assign (segid 3A4 and resid 395 and name O)	(segid 3A4 and resid 396 and name O)	2.26	0.01	0.00
	assign (segid 3A4 and resid 395 and name O)	(segid 3A4 and resid 397 and name C)	3.47	0.11	0.12
	assign (segid 3A4 and resid 395 and name O)	(segid 3A4 and resid 397 and name CA)	4.20	0.15	0.14
	assign (segid 3A4 and resid 395 and name O)	(segid 3A4 and resid 397 and name CB)	4.47	0.16	0.15
60	assign (segid 3A4 and resid 395 and name O)	(segid 3A4 and resid 397 and name N)	5.37	0.20	0.20
	assign (segid 3A4 and resid 395 and name O)	(segid 3A4 and resid 398 and name C)	3.51	0.17	0.17
	assign (segid 3A4 and resid 395 and name O)	(segid 3A4 and resid 398 and name CA)	5.11	0.14	0.14
	assign (segid 3A4 and resid 395 and name O)	(segid 3A4 and resid 398 and name CB)	3.94	0.05	0.05
65	assign (segid 3A4 and resid 395 and name O)	(segid 3A4 and resid 398 and name CD1)	3.93	0.15	0.16
	assign (segid 3A4 and resid 395 and name O)	(segid 3A4 and resid 398 and name CG)	3.93	0.23	0.22
	assign (segid 3A4 and resid 395 and name O)	(segid 3A4 and resid 398 and name N)	5.42	0.29	0.29
	assign (segid 3A4 and resid 395 and name O)	(segid 3A4 and resid 398 and name O)	4.98	0.23	0.22
70	assign (segid 3A4 and resid 395 and name O)	(segid 3A4 and resid 399 and name C)	3.43	0.17	0.17
	assign (segid 3A4 and resid 395 and name O)	(segid 3A4 and resid 399 and name CA)	5.09	0.06	0.06
	assign (segid 3A4 and resid 395 and name O)	(segid 3A4 and resid 399 and name CB)	5.07	0.17	0.16
	assign (segid 3A4 and resid 395 and name O)	(segid 3A4 and resid 399 and name N)	3.89	0.17	0.18
75	assign (segid 3A4 and resid 395 and name O)	(segid 3A4 and resid 399 and name O)	3.53	0.28	0.29
	assign (segid 3A4 and resid 395 and name O)	(segid 3A4 and resid 400 and name C)	3.08	0.09	0.10
	assign (segid 3A4 and resid 395 and name O)	(segid 3A4 and resid 400 and name CA)	6.18	0.14	0.15
	assign (segid 3A4 and resid 395 and name O)	(segid 3A4 and resid 400 and name CB)	7.33	0.14	0.14
	assign (segid 3A4 and resid 395 and name O)	(segid 3A4 and resid 400 and name N)	6.49	0.16	0.16
80	assign (segid 3A4 and resid 395 and name O)	(segid 3A4 and resid 400 and name O)	6.71	0.19	0.20
	assign (segid 3A4 and resid 396 and name C)	(segid 3A4 and resid 401 and name N)	5.13	0.16	0.17
	assign (segid 3A4 and resid 396 and name C)	(segid 3A4 and resid 396 and name CB)	7.03	0.08	0.08
	assign (segid 3A4 and resid 396 and name C)	(segid 3A4 and resid 396 and name N)	2.53	0.02	0.02
	assign (segid 3A4 and resid 396 and name C)	(segid 3A4 and resid 397 and name C)	1.23	0.01	0.01
	assign (segid 3A4 and resid 396 and name C)	(segid 3A4 and resid 397 and name CA)	3.02	0.04	0.03
	assign (segid 3A4 and resid 396 and name C)	(segid 3A4 and resid 397 and name CB)	2.43	0.02	0.01
	assign (segid 3A4 and resid 396 and name C)	(segid 3A4 and resid 397 and name N)	3.68	0.03	0.03
	assign (segid 3A4 and resid 396 and name C)	(segid 3A4 and resid 397 and name O)	1.32	0.02	0.01

	assign (segid 3A4 and resid 396 and name C)	(segid 3A4 and resid 397 and name O)	3.82	0.07	0.07
	assign (segid 3A4 and resid 396 and name C)	(segid 3A4 and resid 398 and name C)	4.60	0.05	0.04
	assign (segid 3A4 and resid 396 and name C)	(segid 3A4 and resid 398 and name CA)	4.52	0.04	0.04
	assign (segid 3A4 and resid 396 and name C)	(segid 3A4 and resid 398 and name CB)	5.34	0.06	0.07
5	assign (segid 3A4 and resid 396 and name C)	(segid 3A4 and resid 398 and name CD1)	7.13	0.12	0.12
	assign (segid 3A4 and resid 396 and name C)	(segid 3A4 and resid 398 and name CG)	6.18	0.04	0.04
	assign (segid 3A4 and resid 396 and name C)	(segid 3A4 and resid 398 and name N)	3.33	0.02	0.03
	assign (segid 3A4 and resid 396 and name C)	(segid 3A4 and resid 398 and name O)	5.70	0.05	0.04
	assign (segid 3A4 and resid 396 and name C)	(segid 3A4 and resid 399 and name C)	4.90	0.06	0.06
10	assign (segid 3A4 and resid 396 and name C)	(segid 3A4 and resid 399 and name CA)	4.57	0.10	0.11
	assign (segid 3A4 and resid 396 and name C)	(segid 3A4 and resid 399 and name CB)	4.35	0.15	0.14
	assign (segid 3A4 and resid 396 and name C)	(segid 3A4 and resid 399 and name N)	3.84	0.10	0.10
	assign (segid 3A4 and resid 396 and name C)	(segid 3A4 and resid 399 and name O)	6.12	0.06	0.06
	assign (segid 3A4 and resid 396 and name C)	(segid 3A4 and resid 400 and name C)	6.12	0.06	0.06
15	assign (segid 3A4 and resid 396 and name C)	(segid 3A4 and resid 400 and name CA)	5.09	0.03	0.04
	assign (segid 3A4 and resid 396 and name C)	(segid 3A4 and resid 400 and name CB)	4.67	0.11	0.11
	assign (segid 3A4 and resid 396 and name C)	(segid 3A4 and resid 400 and name N)	4.18	0.04	0.05
	assign (segid 3A4 and resid 396 and name C)	(segid 3A4 and resid 400 and name O)	7.28	0.06	0.07
	assign (segid 3A4 and resid 396 and name C)	(segid 3A4 and resid 401 and name CA)	7.23	0.05	0.06
20	assign (segid 3A4 and resid 396 and name C)	(segid 3A4 and resid 401 and name N)	5.96	0.06	0.06
	assign (segid 3A4 and resid 396 and name C)	(segid 3A4 and resid 402 and name N)	7.84	0.06	0.06
	assign (segid 3A4 and resid 396 and name C)	(segid HEM and resid 1 and name C1C)	6.85	0.18	0.19
	assign (segid 3A4 and resid 396 and name C)	(segid HEM and resid 1 and name C2C)	6.28	0.28	0.27
	assign (segid 3A4 and resid 396 and name C)	(segid HEM and resid 1 and name C3C)	7.12	0.27	0.27
25	assign (segid 3A4 and resid 396 and name C)	(segid HEM and resid 1 and name C4B)	7.68	0.10	0.11
	assign (segid 3A4 and resid 396 and name C)	(segid HEM and resid 1 and name C4B)	7.35	0.21	0.20
	assign (segid 3A4 and resid 396 and name C)	(segid HEM and resid 1 and name C4C)	6.75	0.17	0.16
	assign (segid 3A4 and resid 396 and name C)	(segid HEM and resid 1 and name C4C)	5.28	0.37	0.37
	assign (segid 3A4 and resid 396 and name CA)	(segid 3A4 and resid 396 and name C)	1.53	0.01	0.02
30	assign (segid 3A4 and resid 396 and name CA)	(segid 3A4 and resid 396 and name CB)	1.54	0.01	0.01
	assign (segid 3A4 and resid 396 and name CA)	(segid 3A4 and resid 396 and name O)	2.40	0.03	0.02
	assign (segid 3A4 and resid 396 and name CA)	(segid 3A4 and resid 397 and name C)	4.42	0.04	0.04
	assign (segid 3A4 and resid 396 and name CA)	(segid 3A4 and resid 397 and name CA)	3.82	0.01	0.02
	assign (segid 3A4 and resid 396 and name CA)	(segid 3A4 and resid 397 and name CB)	4.85	0.02	0.03
35	assign (segid 3A4 and resid 396 and name CA)	(segid 3A4 and resid 397 and name N)	2.45	0.02	0.02
	assign (segid 3A4 and resid 396 and name CA)	(segid 3A4 and resid 397 and name O)	5.29	0.06	0.07
	assign (segid 3A4 and resid 396 and name CA)	(segid 3A4 and resid 398 and name C)	5.55	0.08	0.07
	assign (segid 3A4 and resid 396 and name CA)	(segid 3A4 and resid 398 and name CA)	5.54	0.08	0.07
	assign (segid 3A4 and resid 396 and name CA)	(segid 3A4 and resid 398 and name CB)	6.06	0.12	0.12
40	assign (segid 3A4 and resid 396 and name CA)	(segid 3A4 and resid 398 and name CD1)	7.62	0.18	0.17
	assign (segid 3A4 and resid 396 and name CA)	(segid 3A4 and resid 398 and name CG)	6.92	0.05	0.04
	assign (segid 3A4 and resid 396 and name CA)	(segid 3A4 and resid 398 and name N)	4.45	0.05	0.05
	assign (segid 3A4 and resid 396 and name CA)	(segid 3A4 and resid 398 and name O)	6.68	0.06	0.07
	assign (segid 3A4 and resid 396 and name CA)	(segid 3A4 and resid 399 and name C)	5.72	0.06	0.06
45	assign (segid 3A4 and resid 396 and name CA)	(segid 3A4 and resid 399 and name CA)	5.15	0.12	0.12
	assign (segid 3A4 and resid 396 and name CA)	(segid 3A4 and resid 399 and name CB)	4.49	0.17	0.17
	assign (segid 3A4 and resid 396 and name CA)	(segid 3A4 and resid 399 and name N)	4.59	0.11	0.11
	assign (segid 3A4 and resid 396 and name CA)	(segid 3A4 and resid 399 and name O)	6.93	0.06	0.06
	assign (segid 3A4 and resid 396 and name CA)	(segid 3A4 and resid 400 and name C)	7.35	0.08	0.09
50	assign (segid 3A4 and resid 396 and name CA)	(segid 3A4 and resid 400 and name CA)	6.19	0.05	0.06
	assign (segid 3A4 and resid 396 and name CA)	(segid 3A4 and resid 400 and name CB)	5.85	0.13	0.13
	assign (segid 3A4 and resid 396 and name CA)	(segid 3A4 and resid 400 and name N)	5.19	0.07	0.06
	assign (segid 3A4 and resid 396 and name CA)	(segid 3A4 and resid 401 and name CA)	8.61	0.06	0.06
	assign (segid 3A4 and resid 396 and name CA)	(segid 3A4 and resid 401 and name N)	7.31	0.08	0.08
55	assign (segid 3A4 and resid 396 and name CA)	(segid 3A4 and resid 402 and name CA)	9.98	0.11	0.12
	assign (segid 3A4 and resid 396 and name CA)	(segid 3A4 and resid 402 and name CB)	9.60	0.14	0.14
	assign (segid 3A4 and resid 396 and name CA)	(segid 3A4 and resid 403 and name CA)	10.55	0.17	0.17
	assign (segid 3A4 and resid 396 and name CA)	(segid 3A4 and resid 403 and name CB)	9.75	0.17	0.17
	assign (segid 3A4 and resid 396 and name CA)	(segid 3A4 and resid 404 and name CA)	12.11	0.24	0.24
60	assign (segid 3A4 and resid 396 and name CA)	(segid 3A4 and resid 404 and name CB)	11.66	0.27	0.27
	assign (segid 3A4 and resid 396 and name CA)	(segid 3A4 and resid 405 and name CA)	14.19	0.21	0.21
	assign (segid 3A4 and resid 396 and name CA)	(segid 3A4 and resid 405 and name CB)	13.95	0.23	0.23
	assign (segid 3A4 and resid 396 and name CA)	(segid 3A4 and resid 406 and name CA)	15.34	0.21	0.21
	assign (segid 3A4 and resid 396 and name CA)	(segid 3A4 and resid 407 and name CA)	16.48	0.23	0.22
65	assign (segid 3A4 and resid 396 and name CA)	(segid 3A4 and resid 407 and name CB)	15.76	0.23	0.23
	assign (segid 3A4 and resid 396 and name CA)	(segid 3A4 and resid 408 and name CA)	18.05	0.14	0.15
	assign (segid 3A4 and resid 396 and name CA)	(segid 3A4 and resid 408 and name CB)	17.58	0.13	0.12
	assign (segid 3A4 and resid 396 and name CA)	(segid HEM and resid 1 and name C1C)	7.33	0.22	0.21
70	assign (segid 3A4 and resid 396 and name CA)	(segid HEM and resid 1 and name C2C)	6.64	0.32	0.31
	assign (segid 3A4 and resid 396 and name CA)	(segid HEM and resid 1 and name C3C)	7.22	0.32	0.31
	assign (segid 3A4 and resid 396 and name CA)	(segid HEM and resid 1 and name C4C)	7.47	0.18	0.18
	assign (segid 3A4 and resid 396 and name CA)	(segid HEM and resid 1 and name C4C)	5.79	0.41	0.42
	assign (segid 3A4 and resid 396 and name CB)	(segid 3A4 and resid 397 and name C)	5.47	0.03	0.03
	assign (segid 3A4 and resid 396 and name CB)	(segid 3A4 and resid 397 and name CA)	4.53	0.05	0.05
75	assign (segid 3A4 and resid 396 and name CB)	(segid 3A4 and resid 397 and name CB)	5.39	0.10	0.09
	assign (segid 3A4 and resid 396 and name CB)	(segid 3A4 and resid 397 and name N)	3.20	0.07	0.07
	assign (segid 3A4 and resid 396 and name CB)	(segid 3A4 and resid 397 and name O)	6.29	0.07	0.06
	assign (segid 3A4 and resid 396 and name CB)	(segid 3A4 and resid 398 and name C)	6.97	0.08	0.08
	assign (segid 3A4 and resid 396 and name CB)	(segid 3A4 and resid 398 and name CA)	6.91	0.05	0.06
80	assign (segid 3A4 and resid 396 and name CB)	(segid 3A4 and resid 398 and name CB)	7.50	0.10	0.10
	assign (segid 3A4 and resid 396 and name CB)	(segid 3A4 and resid 398 and name N)	5.71	0.02	0.03
	assign (segid 3A4 and resid 396 and name CB)	(segid 3A4 and resid 399 and name C)	6.88	0.13	0.12
	assign (segid 3A4 and resid 396 and name CB)	(segid 3A4 and resid 399 and name CA)	6.49	0.19	0.18

	assign (segid 3A4 and resid 396 and name CB)	(segid 3A4 and resid 399 and name CB)	5.74	0.26	0.25
	assign (segid 3A4 and resid 396 and name CB)	(segid 3A4 and resid 399 and name N)	6.03	0.14	0.14
	assign (segid 3A4 and resid 396 and name CB)	(segid 3A4 and resid 400 and name CA)	6.95	0.09	0.10
	assign (segid 3A4 and resid 396 and name CB)	(segid 3A4 and resid 400 and name CB)	6.34	0.09	0.10
5	assign (segid 3A4 and resid 396 and name CB)	(segid 3A4 and resid 400 and name N)	6.17	0.13	0.13
	assign (segid 3A4 and resid 396 and name CB)	(segid 3A4 and resid 401 and name CA)	9.60	0.07	0.08
	assign (segid 3A4 and resid 396 and name CB)	(segid 3A4 and resid 402 and name CA)	11.25	0.15	0.15
	assign (segid 3A4 and resid 396 and name CB)	(segid 3A4 and resid 402 and name CB)	10.96	0.16	0.17
	assign (segid 3A4 and resid 396 and name CB)	(segid 3A4 and resid 403 and name CA)	11.54	0.27	0.27
10	assign (segid 3A4 and resid 396 and name CB)	(segid 3A4 and resid 403 and name CB)	10.63	0.28	0.29
	assign (segid 3A4 and resid 396 and name CB)	(segid 3A4 and resid 404 and name CA)	12.87	0.35	0.35
	assign (segid 3A4 and resid 396 and name CB)	(segid 3A4 and resid 404 and name CB)	12.33	0.36	0.37
	assign (segid 3A4 and resid 396 and name CB)	(segid 3A4 and resid 405 and name CA)	15.18	0.30	0.30
	assign (segid 3A4 and resid 396 and name CB)	(segid 3A4 and resid 405 and name CB)	15.02	0.30	0.30
15	assign (segid 3A4 and resid 396 and name CB)	(segid 3A4 and resid 406 and name CA)	16.45	0.29	0.29
	assign (segid 3A4 and resid 396 and name CB)	(segid 3A4 and resid 407 and name CA)	17.34	0.35	0.34
	assign (segid 3A4 and resid 396 and name CB)	(segid 3A4 and resid 407 and name CB)	16.52	0.35	0.35
	assign (segid 3A4 and resid 396 and name CB)	(segid 3A4 and resid 408 and name CA)	18.82	0.25	0.26
	assign (segid 3A4 and resid 396 and name CB)	(segid 3A4 and resid 408 and name CB)	18.33	0.21	0.21
20	assign (segid 3A4 and resid 396 and name CB)	(segid HEM and resid 1 and name C1C)	6.80	0.30	0.31
	assign (segid 3A4 and resid 396 and name CB)	(segid HEM and resid 1 and name C2C)	5.89	0.39	0.39
	assign (segid 3A4 and resid 396 and name CB)	(segid HEM and resid 1 and name C3C)	6.27	0.39	0.40
	assign (segid 3A4 and resid 396 and name CB)	(segid HEM and resid 1 and name C4C)	7.31	0.33	0.34
	assign (segid 3A4 and resid 396 and name CB)	(segid HEM and resid 1 and name CAC)	6.17	0.43	0.43
25	assign (segid 3A4 and resid 396 and name CB)	(segid HEM and resid 1 and name CBC)	5.57	0.53	0.53
	assign (segid 3A4 and resid 396 and name CB)	(segid HEM and resid 1 and name CHC)	7.20	0.28	0.27
	assign (segid 3A4 and resid 396 and name CB)	(segid HEM and resid 1 and name CMC)	5.08	0.48	0.47
	assign (segid 3A4 and resid 396 and name N)	(segid 3A4 and resid 396 and name C)	2.45	0.03	0.03
	assign (segid 3A4 and resid 396 and name N)	(segid 3A4 and resid 396 and name CA)	1.45	0.01	0.02
30	assign (segid 3A4 and resid 396 and name N)	(segid 3A4 and resid 396 and name CB)	2.47	0.02	0.01
	assign (segid 3A4 and resid 396 and name N)	(segid 3A4 and resid 396 and name O)	3.47	0.06	0.06
	assign (segid 3A4 and resid 396 and name N)	(segid 3A4 and resid 397 and name C)	4.71	0.04	0.04
	assign (segid 3A4 and resid 396 and name N)	(segid 3A4 and resid 397 and name CA)	4.21	0.01	0.02
	assign (segid 3A4 and resid 396 and name N)	(segid 3A4 and resid 397 and name CB)	4.93	0.02	0.02
35	assign (segid 3A4 and resid 396 and name N)	(segid 3A4 and resid 397 and name N)	2.82	0.03	0.03
	assign (segid 3A4 and resid 396 and name N)	(segid 3A4 and resid 397 and name O)	5.77	0.06	0.07
	assign (segid 3A4 and resid 396 and name N)	(segid 3A4 and resid 398 and name C)	5.68	0.03	0.03
	assign (segid 3A4 and resid 396 and name N)	(segid 3A4 and resid 398 and name CA)	5.42	0.04	0.04
	assign (segid 3A4 and resid 396 and name N)	(segid 3A4 and resid 398 and name CB)	5.60	0.07	0.07
40	assign (segid 3A4 and resid 396 and name N)	(segid 3A4 and resid 398 and name CD1)	6.77	0.17	0.16
	assign (segid 3A4 and resid 396 and name N)	(segid 3A4 and resid 398 and name CG)	6.29	0.04	0.05
	assign (segid 3A4 and resid 396 and name N)	(segid 3A4 and resid 398 and name N)	4.39	0.04	0.03
	assign (segid 3A4 and resid 396 and name N)	(segid 3A4 and resid 398 and name O)	6.89	0.04	0.03
	assign (segid 3A4 and resid 396 and name N)	(segid 3A4 and resid 399 and name C)	6.47	0.07	0.07
45	assign (segid 3A4 and resid 396 and name N)	(segid 3A4 and resid 399 and name CA)	5.62	0.07	0.06
	assign (segid 3A4 and resid 396 and name N)	(segid 3A4 and resid 399 and name CB)	5.03	0.11	0.11
	assign (segid 3A4 and resid 396 and name N)	(segid 3A4 and resid 399 and name N)	4.84	0.04	0.05
	assign (segid 3A4 and resid 396 and name N)	(segid 3A4 and resid 399 and name O)	7.67	0.06	0.07
	assign (segid 3A4 and resid 396 and name N)	(segid 3A4 and resid 400 and name CA)	7.26	0.08	0.07
50	assign (segid 3A4 and resid 396 and name N)	(segid 3A4 and resid 400 and name CB)	7.03	0.14	0.14
	assign (segid 3A4 and resid 396 and name N)	(segid 3A4 and resid 400 and name N)	6.12	0.07	0.07
	assign (segid 3A4 and resid 396 and name N)	(segid HEM and resid 1 and name C1C)	7.38	0.22	0.22
	assign (segid 3A4 and resid 396 and name N)	(segid HEM and resid 1 and name C2C)	6.89	0.33	0.32
	assign (segid 3A4 and resid 396 and name N)	(segid HEM and resid 1 and name CHC)	7.53	0.19	0.19
55	assign (segid 3A4 and resid 396 and name N)	(segid HEM and resid 1 and name CMC)	6.33	0.42	0.42
	assign (segid 3A4 and resid 396 and name O)	(segid 3A4 and resid 396 and name CB)	3.32	0.08	0.08
	assign (segid 3A4 and resid 396 and name O)	(segid 3A4 and resid 397 and name C)	2.95	0.04	0.03
	assign (segid 3A4 and resid 396 and name O)	(segid 3A4 and resid 397 and name CA)	2.75	0.03	0.04
	assign (segid 3A4 and resid 396 and name O)	(segid 3A4 and resid 397 and name CB)	4.22	0.05	0.05
60	assign (segid 3A4 and resid 396 and name O)	(segid 3A4 and resid 397 and name N)	2.23	0.02	0.02
	assign (segid 3A4 and resid 396 and name O)	(segid 3A4 and resid 397 and name O)	3.38	0.09	0.09
	assign (segid 3A4 and resid 396 and name O)	(segid 3A4 and resid 398 and name C)	4.13	0.07	0.08
	assign (segid 3A4 and resid 396 and name O)	(segid 3A4 and resid 398 and name CA)	4.39	0.06	0.07
	assign (segid 3A4 and resid 396 and name O)	(segid 3A4 and resid 398 and name CB)	5.44	0.06	0.06
65	assign (segid 3A4 and resid 396 and name O)	(segid 3A4 and resid 398 and name CD1)	7.51	0.11	0.12
	assign (segid 3A4 and resid 396 and name O)	(segid 3A4 and resid 398 and name CG)	6.46	0.10	0.09
	assign (segid 3A4 and resid 396 and name O)	(segid 3A4 and resid 398 and name N)	3.45	0.05	0.04
	assign (segid 3A4 and resid 396 and name O)	(segid 3A4 and resid 398 and name O)	5.08	0.10	0.10
	assign (segid 3A4 and resid 396 and name O)	(segid 3A4 and resid 399 and name C)	3.85	0.08	0.07
70	assign (segid 3A4 and resid 396 and name O)	(segid 3A4 and resid 399 and name CA)	3.79	0.10	0.10
	assign (segid 3A4 and resid 396 and name O)	(segid 3A4 and resid 399 and name CB)	3.67	0.12	0.11
	assign (segid 3A4 and resid 396 and name O)	(segid 3A4 and resid 399 and name N)	3.31	0.10	0.09
	assign (segid 3A4 and resid 396 and name O)	(segid 3A4 and resid 399 and name O)	5.04	0.05	0.05
	assign (segid 3A4 and resid 396 and name O)	(segid 3A4 and resid 400 and name C)	5.00	0.07	0.07
75	assign (segid 3A4 and resid 396 and name O)	(segid 3A4 and resid 400 and name CA)	3.90	0.04	0.03
	assign (segid 3A4 and resid 396 and name O)	(segid 3A4 and resid 400 and name CB)	3.57	0.13	0.13
	assign (segid 3A4 and resid 396 and name O)	(segid 3A4 and resid 400 and name N)	3.02	0.05	0.05
	assign (segid 3A4 and resid 396 and name O)	(segid 3A4 and resid 400 and name O)	6.14	0.07	0.07
	assign (segid 3A4 and resid 396 and name O)	(segid 3A4 and resid 401 and name C)	7.21	0.07	0.06
80	assign (segid 3A4 and resid 396 and name O)	(segid 3A4 and resid 401 and name CA)	6.34	0.07	0.07
	assign (segid 3A4 and resid 396 and name O)	(segid 3A4 and resid 401 and name N)	4.99	0.08	0.07
	assign (segid 3A4 and resid 396 and name O)	(segid 3A4 and resid 402 and name N)	6.93	0.09	0.08
	assign (segid 3A4 and resid 396 and name O)	(segid 3A4 and resid 403 and name CB)	7.87	0.09	0.09

	assign (segid 3A4 and resid 396 and name O)	(segid 3A4 and resid 403 and name N)	7.80	0.08	0.08
	assign (segid 3A4 and resid 396 and name O)	(segid HEM and resid 1 and name C2C)	7.05	0.27	0.27
	assign (segid 3A4 and resid 396 and name O)	(segid HEM and resid 1 and name CHC)	7.46	0.18	0.18
	assign (segid 3A4 and resid 396 and name O)	(segid HEM and resid 1 and name CMC)	5.88	0.35	0.34
5	assign (segid 3A4 and resid 397 and name C)	(segid 3A4 and resid 397 and name CB)	2.46	0.03	0.04
	assign (segid 3A4 and resid 397 and name C)	(segid 3A4 and resid 397 and name O)	1.24	0.01	0.01
	assign (segid 3A4 and resid 397 and name C)	(segid 3A4 and resid 398 and name C)	3.06	0.04	0.03
	assign (segid 3A4 and resid 397 and name C)	(segid 3A4 and resid 398 and name CA)	2.42	0.01	0.02
	assign (segid 3A4 and resid 397 and name C)	(segid 3A4 and resid 398 and name CB)	3.69	0.04	0.03
10	assign (segid 3A4 and resid 397 and name C)	(segid 3A4 and resid 398 and name CD1)	5.61	0.09	0.08
	assign (segid 3A4 and resid 397 and name C)	(segid 3A4 and resid 398 and name CG)	4.26	0.08	0.09
	assign (segid 3A4 and resid 397 and name C)	(segid 3A4 and resid 398 and name N)	1.32	0.01	0.02
	assign (segid 3A4 and resid 397 and name C)	(segid 3A4 and resid 398 and name O)	3.95	0.04	0.05
	assign (segid 3A4 and resid 397 and name C)	(segid 3A4 and resid 399 and name C)	4.59	0.12	0.11
15	assign (segid 3A4 and resid 397 and name C)	(segid 3A4 and resid 399 and name CA)	4.49	0.09	0.09
	assign (segid 3A4 and resid 397 and name C)	(segid 3A4 and resid 399 and name CB)	5.22	0.08	0.08
	assign (segid 3A4 and resid 397 and name C)	(segid 3A4 and resid 399 and name N)	3.29	0.09	0.09
	assign (segid 3A4 and resid 397 and name C)	(segid 3A4 and resid 399 and name O)	5.59	0.17	0.18
	assign (segid 3A4 and resid 397 and name C)	(segid 3A4 and resid 400 and name C)	4.96	0.05	0.05
20	assign (segid 3A4 and resid 397 and name C)	(segid 3A4 and resid 400 and name CA)	4.70	0.13	0.13
	assign (segid 3A4 and resid 397 and name C)	(segid 3A4 and resid 400 and name CB)	4.52	0.23	0.22
	assign (segid 3A4 and resid 397 and name C)	(segid 3A4 and resid 400 and name N)	3.98	0.11	0.11
	assign (segid 3A4 and resid 397 and name C)	(segid 3A4 and resid 400 and name O)	6.17	0.04	0.04
	assign (segid 3A4 and resid 397 and name C)	(segid 3A4 and resid 401 and name C)	6.11	0.08	0.08
25	assign (segid 3A4 and resid 397 and name C)	(segid 3A4 and resid 401 and name CA)	5.08	0.07	0.06
	assign (segid 3A4 and resid 397 and name C)	(segid 3A4 and resid 401 and name N)	4.20	0.05	0.04
	assign (segid 3A4 and resid 397 and name C)	(segid 3A4 and resid 401 and name O)	7.28	0.08	0.08
	assign (segid 3A4 and resid 397 and name C)	(segid 3A4 and resid 402 and name CA)	7.22	0.07	0.06
	assign (segid 3A4 and resid 397 and name C)	(segid 3A4 and resid 402 and name CB)	7.20	0.08	0.08
30	assign (segid 3A4 and resid 397 and name C)	(segid 3A4 and resid 402 and name N)	5.95	0.06	0.06
	assign (segid 3A4 and resid 397 and name C)	(segid 3A4 and resid 403 and name N)	7.83	0.06	0.06
	assign (segid 3A4 and resid 397 and name C)	(segid HEM and resid 1 and name C1C)	7.14	0.22	0.21
	assign (segid 3A4 and resid 397 and name C)	(segid HEM and resid 1 and name C2C)	7.08	0.27	0.26
	assign (segid 3A4 and resid 397 and name C)	(segid HEM and resid 1 and name C3B)	6.69	0.20	0.21
35	assign (segid 3A4 and resid 397 and name C)	(segid HEM and resid 1 and name C4B)	6.96	0.19	0.20
	assign (segid 3A4 and resid 397 and name C)	(segid HEM and resid 1 and name CAB)	5.77	0.21	0.21
	assign (segid 3A4 and resid 397 and name C)	(segid HEM and resid 1 and name CBB)	5.72	0.25	0.25
	assign (segid 3A4 and resid 397 and name C)	(segid HEM and resid 1 and name CHC)	6.45	0.21	0.21
	assign (segid 3A4 and resid 397 and name C)	(segid HEM and resid 1 and name CMC)	6.16	0.31	0.32
40	assign (segid 3A4 and resid 397 and name CA)	(segid 3A4 and resid 397 and name C)	1.52	0.01	0.01
	assign (segid 3A4 and resid 397 and name CA)	(segid 3A4 and resid 397 and name CB)	1.50	0.01	0.02
	assign (segid 3A4 and resid 397 and name CA)	(segid 3A4 and resid 397 and name O)	2.38	0.04	0.03
	assign (segid 3A4 and resid 397 and name CA)	(segid 3A4 and resid 398 and name C)	4.45	0.03	0.03
	assign (segid 3A4 and resid 397 and name CA)	(segid 3A4 and resid 398 and name CA)	3.81	0.01	0.01
45	assign (segid 3A4 and resid 397 and name CA)	(segid 3A4 and resid 398 and name CB)	4.86	0.03	0.03
	assign (segid 3A4 and resid 397 and name CA)	(segid 3A4 and resid 398 and name CD1)	6.49	0.11	0.10
	assign (segid 3A4 and resid 397 and name CA)	(segid 3A4 and resid 398 and name CG)	5.26	0.08	0.08
	assign (segid 3A4 and resid 397 and name CA)	(segid 3A4 and resid 398 and name N)	2.45	0.02	0.01
	assign (segid 3A4 and resid 397 and name CA)	(segid 3A4 and resid 398 and name O)	5.41	0.04	0.04
50	assign (segid 3A4 and resid 397 and name CA)	(segid 3A4 and resid 399 and name C)	5.54	0.09	0.10
	assign (segid 3A4 and resid 397 and name CA)	(segid 3A4 and resid 399 and name CA)	5.48	0.08	0.09
	assign (segid 3A4 and resid 397 and name CA)	(segid 3A4 and resid 399 and name CB)	5.89	0.11	0.10
	assign (segid 3A4 and resid 397 and name CA)	(segid 3A4 and resid 399 and name N)	4.39	0.08	0.09
	assign (segid 3A4 and resid 397 and name CA)	(segid 3A4 and resid 399 and name O)	6.64	0.14	0.13
55	assign (segid 3A4 and resid 397 and name CA)	(segid 3A4 and resid 400 and name C)	5.80	0.05	0.05
	assign (segid 3A4 and resid 397 and name CA)	(segid 3A4 and resid 400 and name CA)	5.29	0.09	0.10
	assign (segid 3A4 and resid 397 and name CA)	(segid 3A4 and resid 400 and name CB)	4.70	0.20	0.19
	assign (segid 3A4 and resid 397 and name CA)	(segid 3A4 and resid 400 and name N)	4.71	0.07	0.07
	assign (segid 3A4 and resid 397 and name CA)	(segid 3A4 and resid 400 and name O)	6.99	0.06	0.06
60	assign (segid 3A4 and resid 397 and name CA)	(segid 3A4 and resid 401 and name C)	7.36	0.10	0.10
	assign (segid 3A4 and resid 397 and name CA)	(segid 3A4 and resid 401 and name CA)	6.19	0.08	0.09
	assign (segid 3A4 and resid 397 and name CA)	(segid 3A4 and resid 401 and name N)	5.22	0.07	0.07
	assign (segid 3A4 and resid 397 and name CA)	(segid 3A4 and resid 402 and name CA)	8.62	0.08	0.07
	assign (segid 3A4 and resid 397 and name CA)	(segid 3A4 and resid 402 and name CB)	8.64	0.10	0.09
65	assign (segid 3A4 and resid 397 and name CA)	(segid 3A4 and resid 402 and name N)	7.31	0.07	0.08
	assign (segid 3A4 and resid 397 and name CA)	(segid 3A4 and resid 403 and name CA)	10.02	0.08	0.07
	assign (segid 3A4 and resid 397 and name CA)	(segid 3A4 and resid 403 and name CB)	9.65	0.10	0.10
	assign (segid 3A4 and resid 397 and name CA)	(segid 3A4 and resid 404 and name CA)	10.64	0.11	0.10
	assign (segid 3A4 and resid 397 and name CA)	(segid 3A4 and resid 404 and name CB)	9.87	0.12	0.11
70	assign (segid 3A4 and resid 397 and name CA)	(segid 3A4 and resid 405 and name CA)	12.19	0.21	0.20
	assign (segid 3A4 and resid 397 and name CA)	(segid 3A4 and resid 405 and name CB)	11.73	0.23	0.23
	assign (segid 3A4 and resid 397 and name CA)	(segid 3A4 and resid 406 and name CA)	14.13	0.22	0.21
	assign (segid 3A4 and resid 397 and name CA)	(segid 3A4 and resid 407 and name CA)	15.52	0.15	0.14
	assign (segid 3A4 and resid 397 and name CA)	(segid 3A4 and resid 407 and name CB)	14.99	0.11	0.11
75	assign (segid 3A4 and resid 397 and name CA)	(segid 3A4 and resid 408 and name CA)	16.38	0.05	0.05
	assign (segid 3A4 and resid 397 and name CA)	(segid 3A4 and resid 408 and name CB)	15.64	0.07	0.07
	assign (segid 3A4 and resid 397 and name CA)	(segid 3A4 and resid 409 and name CA)	18.34	0.39	0.38
	assign (segid 3A4 and resid 397 and name CA)	(segid 3A4 and resid 409 and name CB)	17.95	0.55	0.55
	assign (segid 3A4 and resid 397 and name CA)	(segid 3A4 and resid 433 and name CA)	16.35	0.48	0.49
80	assign (segid 3A4 and resid 397 and name CA)	(segid 3A4 and resid 434 and name CA)	15.97	0.62	0.62
	assign (segid 3A4 and resid 397 and name CA)	(segid 3A4 and resid 435 and name CA)	17.76	0.52	0.52
	assign (segid 3A4 and resid 397 and name CA)	(segid HEM and resid 1 and name C1B)	7.67	0.17	0.16
	assign (segid 3A4 and resid 397 and name CA)	(segid HEM and resid 1 and name C1C)	5.76	0.19	0.18

	assign (segid 3A4 and resid 397 and name CA)	(segid HEM and resid 1 and name C2B)	7.05	0.15	0.14
	assign (segid 3A4 and resid 397 and name CA)	(segid HEM and resid 1 and name C2C)	5.59	0.25	0.26
	assign (segid 3A4 and resid 397 and name CA)	(segid HEM and resid 1 and name C3B)	5.90	0.16	0.15
	assign (segid 3A4 and resid 397 and name CA)	(segid HEM and resid 1 and name C3C)	6.74	0.23	0.24
5	assign (segid 3A4 and resid 397 and name CA)	(segid HEM and resid 1 and name C4B)	5.91	0.15	0.15
	assign (segid 3A4 and resid 397 and name CA)	(segid HEM and resid 1 and name C4C)	7.45	0.21	0.20
	assign (segid 3A4 and resid 397 and name CA)	(segid HEM and resid 1 and name CAB)	5.11	0.20	0.19
	assign (segid 3A4 and resid 397 and name CA)	(segid HEM and resid 1 and name CAC)	7.48	0.25	0.25
	assign (segid 3A4 and resid 397 and name CA)	(segid HEM and resid 1 and name CBB)	5.38	0.25	0.25
10	assign (segid 3A4 and resid 397 and name CA)	(segid HEM and resid 1 and name CHC)	5.21	0.17	0.17
	assign (segid 3A4 and resid 397 and name CA)	(segid HEM and resid 1 and name CMC)	4.67	0.31	0.32
	assign (segid 3A4 and resid 397 and name CA)	(segid HEM and resid 1 and name NB)	7.07	0.17	0.16
	assign (segid 3A4 and resid 397 and name CA)	(segid HEM and resid 1 and name NC)	6.93	0.18	0.17
	assign (segid 3A4 and resid 397 and name CB)	(segid 3A4 and resid 398 and name C)	5.42	0.03	0.03
15	assign (segid 3A4 and resid 397 and name CB)	(segid 3A4 and resid 398 and name CA)	4.42	0.02	0.02
	assign (segid 3A4 and resid 397 and name CB)	(segid 3A4 and resid 398 and name CB)	5.24	0.03	0.03
	assign (segid 3A4 and resid 397 and name CB)	(segid 3A4 and resid 398 and name CD1)	6.36	0.12	0.12
	assign (segid 3A4 and resid 397 and name CB)	(segid 3A4 and resid 398 and name CG)	5.19	0.10	0.11
	assign (segid 3A4 and resid 397 and name CB)	(segid 3A4 and resid 398 and name N)	3.11	0.02	0.02
20	assign (segid 3A4 and resid 397 and name CB)	(segid 3A4 and resid 398 and name O)	6.34	0.04	0.04
	assign (segid 3A4 and resid 397 and name CB)	(segid 3A4 and resid 399 and name C)	6.92	0.09	0.10
	assign (segid 3A4 and resid 397 and name CB)	(segid 3A4 and resid 399 and name CA)	6.80	0.07	0.07
	assign (segid 3A4 and resid 397 and name CB)	(segid 3A4 and resid 399 and name CB)	7.26	0.08	0.09
	assign (segid 3A4 and resid 397 and name CB)	(segid 3A4 and resid 399 and name N)	5.58	0.07	0.06
25	assign (segid 3A4 and resid 397 and name CB)	(segid 3A4 and resid 400 and name C)	6.98	0.06	0.05
	assign (segid 3A4 and resid 397 and name CB)	(segid 3A4 and resid 400 and name CA)	6.65	0.11	0.10
	assign (segid 3A4 and resid 397 and name CB)	(segid 3A4 and resid 400 and name CB)	5.99	0.22	0.21
	assign (segid 3A4 and resid 397 and name CB)	(segid 3A4 and resid 400 and name N)	6.14	0.08	0.07
	assign (segid 3A4 and resid 397 and name CB)	(segid 3A4 and resid 401 and name CA)	6.99	0.10	0.09
30	assign (segid 3A4 and resid 397 and name CB)	(segid 3A4 and resid 401 and name N)	6.23	0.07	0.08
	assign (segid 3A4 and resid 397 and name CB)	(segid 3A4 and resid 402 and name CA)	9.56	0.09	0.10
	assign (segid 3A4 and resid 397 and name CB)	(segid 3A4 and resid 402 and name CB)	9.60	0.10	0.10
	assign (segid 3A4 and resid 397 and name CB)	(segid 3A4 and resid 403 and name CA)	11.27	0.07	0.08
	assign (segid 3A4 and resid 397 and name CB)	(segid 3A4 and resid 403 and name CB)	11.01	0.11	0.11
35	assign (segid 3A4 and resid 397 and name CB)	(segid 3A4 and resid 404 and name CA)	11.69	0.09	0.08
	assign (segid 3A4 and resid 397 and name CB)	(segid 3A4 and resid 404 and name CB)	10.81	0.08	0.09
	assign (segid 3A4 and resid 397 and name CB)	(segid 3A4 and resid 405 and name CA)	12.97	0.22	0.21
	assign (segid 3A4 and resid 397 and name CB)	(segid 3A4 and resid 405 and name CB)	12.39	0.23	0.23
	assign (segid 3A4 and resid 397 and name CB)	(segid 3A4 and resid 406 and name CA)	15.12	0.23	0.22
40	assign (segid 3A4 and resid 397 and name CB)	(segid 3A4 and resid 407 and name CA)	16.63	0.13	0.14
	assign (segid 3A4 and resid 397 and name CB)	(segid 3A4 and resid 407 and name CB)	16.17	0.08	0.09
	assign (segid 3A4 and resid 397 and name CB)	(segid 3A4 and resid 408 and name CA)	17.27	0.06	0.07
	assign (segid 3A4 and resid 397 and name CB)	(segid 3A4 and resid 408 and name CB)	16.44	0.09	0.09
	assign (segid 3A4 and resid 397 and name CB)	(segid 3A4 and resid 431 and name CA)	17.08	1.04	1.04
45	assign (segid 3A4 and resid 397 and name CB)	(segid 3A4 and resid 433 and name CA)	15.29	0.48	0.48
	assign (segid 3A4 and resid 397 and name CB)	(segid 3A4 and resid 434 and name CA)	15.16	0.61	0.60
	assign (segid 3A4 and resid 397 and name CB)	(segid 3A4 and resid 435 and name CA)	17.18	0.51	0.51
	assign (segid 3A4 and resid 397 and name CB)	(segid HEM and resid 1 and name C1B)	6.20	0.18	0.18
	assign (segid 3A4 and resid 397 and name CB)	(segid HEM and resid 1 and name C1C)	4.79	0.21	0.22
50	assign (segid 3A4 and resid 397 and name CB)	(segid HEM and resid 1 and name C2B)	5.59	0.14	0.14
	assign (segid 3A4 and resid 397 and name CB)	(segid HEM and resid 1 and name C2C)	4.98	0.27	0.27
	assign (segid 3A4 and resid 397 and name CB)	(segid HEM and resid 1 and name C3B)	4.49	0.14	0.15
	assign (segid 3A4 and resid 397 and name CB)	(segid HEM and resid 1 and name C3C)	6.18	0.25	0.25
	assign (segid 3A4 and resid 397 and name CB)	(segid HEM and resid 1 and name C4B)	4.56	0.17	0.17
55	assign (segid 3A4 and resid 397 and name CB)	(segid HEM and resid 1 and name C4C)	6.64	0.23	0.22
	assign (segid 3A4 and resid 397 and name CB)	(segid HEM and resid 1 and name CAB)	3.83	0.18	0.18
	assign (segid 3A4 and resid 397 and name CB)	(segid HEM and resid 1 and name CAC)	7.15	0.25	0.26
	assign (segid 3A4 and resid 397 and name CB)	(segid HEM and resid 1 and name CBB)	4.25	0.26	0.25
	assign (segid 3A4 and resid 397 and name CB)	(segid HEM and resid 1 and name CHB)	7.44	0.19	0.18
60	assign (segid 3A4 and resid 397 and name CB)	(segid HEM and resid 1 and name CHC)	4.05	0.20	0.21
	assign (segid 3A4 and resid 397 and name CB)	(segid HEM and resid 1 and name CMB)	6.44	0.17	0.17
	assign (segid 3A4 and resid 397 and name CB)	(segid HEM and resid 1 and name CMC)	4.40	0.31	0.31
	assign (segid 3A4 and resid 397 and name CB)	(segid HEM and resid 1 and name FE)	6.75	0.11	0.12
	assign (segid 3A4 and resid 397 and name CB)	(segid HEM and resid 1 and name NB)	5.68	0.20	0.19
65	assign (segid 3A4 and resid 397 and name CB)	(segid HEM and resid 1 and name NC)	5.91	0.21	0.20
	assign (segid 3A4 and resid 397 and name N)	(segid 3A4 and resid 397 and name C)	2.46	0.03	0.02
	assign (segid 3A4 and resid 397 and name N)	(segid 3A4 and resid 397 and name CA)	1.46	0.02	0.01
	assign (segid 3A4 and resid 397 and name N)	(segid 3A4 and resid 397 and name CB)	2.43	0.03	0.02
	assign (segid 3A4 and resid 397 and name N)	(segid 3A4 and resid 397 and name O)	3.47	0.04	0.04
70	assign (segid 3A4 and resid 397 and name N)	(segid 3A4 and resid 398 and name C)	4.75	0.05	0.05
	assign (segid 3A4 and resid 397 and name N)	(segid 3A4 and resid 398 and name CA)	4.25	0.05	0.05
	assign (segid 3A4 and resid 397 and name N)	(segid 3A4 and resid 398 and name CB)	5.05	0.08	0.08
	assign (segid 3A4 and resid 397 and name N)	(segid 3A4 and resid 398 and name CD1)	6.59	0.14	0.15
	assign (segid 3A4 and resid 397 and name N)	(segid 3A4 and resid 398 and name CG)	5.59	0.03	0.03
75	assign (segid 3A4 and resid 397 and name N)	(segid 3A4 and resid 398 and name N)	2.85	0.05	0.05
	assign (segid 3A4 and resid 397 and name N)	(segid 3A4 and resid 398 and name O)	5.86	0.04	0.04
	assign (segid 3A4 and resid 397 and name N)	(segid 3A4 and resid 399 and name C)	5.65	0.06	0.07
	assign (segid 3A4 and resid 397 and name N)	(segid 3A4 and resid 399 and name CA)	5.34	0.10	0.09
	assign (segid 3A4 and resid 397 and name N)	(segid 3A4 and resid 399 and name CB)	5.38	0.13	0.12
80	assign (segid 3A4 and resid 397 and name N)	(segid 3A4 and resid 399 and name N)	4.32	0.10	0.11
	assign (segid 3A4 and resid 397 and name N)	(segid 3A4 and resid 399 and name O)	6.84	0.08	0.09
	assign (segid 3A4 and resid 397 and name N)	(segid 3A4 and resid 400 and name C)	6.50	0.06	0.06
	assign (segid 3A4 and resid 397 and name N)	(segid 3A4 and resid 400 and name CA)	5.71	0.05	0.04

	assign (segid 3A4 and resid 397 and name N)	(segid 3A4 and resid 400 and name CB)	5.17	0.13	0.13
	assign (segid 3A4 and resid 397 and name N)	(segid 3A4 and resid 400 and name N)	4.91	0.04	0.03
	assign (segid 3A4 and resid 397 and name N)	(segid 3A4 and resid 400 and name O)	7.70	0.07	0.07
	assign (segid 3A4 and resid 397 and name N)	(segid 3A4 and resid 401 and name CA)	7.23	0.07	0.07
5	assign (segid 3A4 and resid 397 and name N)	(segid 3A4 and resid 401 and name N)	6.11	0.07	0.07
	assign (segid 3A4 and resid 397 and name N)	(segid HEM and resid 1 and name C1C)	5.84	0.19	0.18
	assign (segid 3A4 and resid 397 and name N)	(segid HEM and resid 1 and name C2B)	7.83	0.08	0.08
	assign (segid 3A4 and resid 397 and name N)	(segid HEM and resid 1 and name C2C)	5.47	0.27	0.28
	assign (segid 3A4 and resid 397 and name N)	(segid HEM and resid 1 and name C3B)	6.71	0.11	0.11
10	assign (segid 3A4 and resid 397 and name N)	(segid HEM and resid 1 and name C3C)	6.42	0.26	0.26
	assign (segid 3A4 and resid 397 and name N)	(segid HEM and resid 1 and name C4B)	6.46	0.10	0.10
	assign (segid 3A4 and resid 397 and name N)	(segid HEM and resid 1 and name C4C)	7.19	0.20	0.20
	assign (segid 3A4 and resid 397 and name N)	(segid HEM and resid 1 and name CAB)	6.14	0.19	0.19
	assign (segid 3A4 and resid 397 and name N)	(segid HEM and resid 1 and name CAC)	6.98	0.28	0.27
15	assign (segid 3A4 and resid 397 and name N)	(segid HEM and resid 1 and name CBB)	6.60	0.23	0.24
	assign (segid 3A4 and resid 397 and name N)	(segid HEM and resid 1 and name CBC)	6.84	0.48	0.48
	assign (segid 3A4 and resid 397 and name N)	(segid HEM and resid 1 and name CHC)	5.61	0.16	0.16
	assign (segid 3A4 and resid 397 and name N)	(segid HEM and resid 1 and name CHC)	4.62	0.37	0.36
	assign (segid 3A4 and resid 397 and name N)	(segid HEM and resid 1 and name NC)	7.47	0.10	0.10
20	assign (segid 3A4 and resid 397 and name N)	(segid HEM and resid 1 and name NB)	6.88	0.15	0.15
	assign (segid 3A4 and resid 397 and name O)	(segid 3A4 and resid 397 and name CB)	3.27	0.05	0.06
	assign (segid 3A4 and resid 397 and name O)	(segid 3A4 and resid 398 and name C)	3.04	0.06	0.05
	assign (segid 3A4 and resid 397 and name O)	(segid 3A4 and resid 398 and name CA)	2.75	0.05	0.05
	assign (segid 3A4 and resid 397 and name O)	(segid 3A4 and resid 398 and name CB)	4.22	0.07	0.06
25	assign (segid 3A4 and resid 397 and name O)	(segid 3A4 and resid 398 and name CD1)	6.29	0.11	0.10
	assign (segid 3A4 and resid 397 and name O)	(segid 3A4 and resid 398 and name CG)	4.85	0.10	0.10
	assign (segid 3A4 and resid 397 and name O)	(segid 3A4 and resid 398 and name N)	2.24	0.01	0.02
	assign (segid 3A4 and resid 397 and name O)	(segid 3A4 and resid 398 and name O)	3.59	0.05	0.04
	assign (segid 3A4 and resid 397 and name O)	(segid 3A4 and resid 399 and name C)	4.16	0.18	0.18
30	assign (segid 3A4 and resid 397 and name O)	(segid 3A4 and resid 399 and name CA)	4.43	0.14	0.15
	assign (segid 3A4 and resid 397 and name O)	(segid 3A4 and resid 399 and name CB)	5.38	0.14	0.13
	assign (segid 3A4 and resid 397 and name O)	(segid 3A4 and resid 399 and name N)	3.45	0.12	0.13
	assign (segid 3A4 and resid 397 and name O)	(segid 3A4 and resid 399 and name O)	5.00	0.24	0.23
	assign (segid 3A4 and resid 397 and name O)	(segid 3A4 and resid 400 and name C)	3.93	0.08	0.08
35	assign (segid 3A4 and resid 397 and name O)	(segid 3A4 and resid 400 and name CA)	3.93	0.19	0.19
	assign (segid 3A4 and resid 397 and name O)	(segid 3A4 and resid 400 and name CB)	3.82	0.27	0.28
	assign (segid 3A4 and resid 397 and name O)	(segid 3A4 and resid 400 and name N)	3.48	0.17	0.17
	assign (segid 3A4 and resid 397 and name O)	(segid 3A4 and resid 400 and name O)	5.10	0.06	0.05
	assign (segid 3A4 and resid 397 and name O)	(segid 3A4 and resid 401 and name C)	5.02	0.08	0.08
40	assign (segid 3A4 and resid 397 and name O)	(segid 3A4 and resid 401 and name CA)	3.89	0.06	0.06
	assign (segid 3A4 and resid 397 and name O)	(segid 3A4 and resid 401 and name N)	3.06	0.05	0.04
	assign (segid 3A4 and resid 397 and name O)	(segid 3A4 and resid 401 and name O)	6.15	0.08	0.08
	assign (segid 3A4 and resid 397 and name O)	(segid 3A4 and resid 402 and name C)	7.27	0.05	0.04
	assign (segid 3A4 and resid 397 and name O)	(segid 3A4 and resid 402 and name CA)	6.39	0.07	0.07
45	assign (segid 3A4 and resid 397 and name O)	(segid 3A4 and resid 402 and name CB)	6.59	0.09	0.08
	assign (segid 3A4 and resid 397 and name O)	(segid 3A4 and resid 402 and name N)	5.02	0.06	0.07
	assign (segid 3A4 and resid 397 and name O)	(segid 3A4 and resid 403 and name N)	6.97	0.09	0.10
	assign (segid 3A4 and resid 397 and name O)	(segid HEM and resid 1 and name C3B)	7.10	0.24	0.25
	assign (segid 3A4 and resid 397 and name O)	(segid HEM and resid 1 and name C4B)	7.53	0.22	0.21
50	assign (segid 3A4 and resid 397 and name O)	(segid HEM and resid 1 and name CAB)	5.99	0.24	0.25
	assign (segid 3A4 and resid 397 and name O)	(segid HEM and resid 1 and name CBB)	5.74	0.29	0.28
	assign (segid 3A4 and resid 397 and name O)	(segid HEM and resid 1 and name CHC)	7.04	0.20	0.20
	assign (segid 3A4 and resid 397 and name O)	(segid HEM and resid 1 and name CHC)	6.71	0.28	0.28
	assign (segid 3A4 and resid 397 and name O)	(segid HEM and resid 1 and name CHC)	2.48	0.02	0.02
55	assign (segid 3A4 and resid 398 and name C)	(segid 3A4 and resid 398 and name CD1)	4.94	0.07	0.07
	assign (segid 3A4 and resid 398 and name C)	(segid 3A4 and resid 398 and name CG)	3.85	0.02	0.02
	assign (segid 3A4 and resid 398 and name C)	(segid 3A4 and resid 398 and name O)	1.24	0.01	0.00
	assign (segid 3A4 and resid 398 and name C)	(segid 3A4 and resid 399 and name C)	3.04	0.04	0.04
	assign (segid 3A4 and resid 398 and name C)	(segid 3A4 and resid 399 and name CA)	2.44	0.01	0.01
60	assign (segid 3A4 and resid 398 and name C)	(segid 3A4 and resid 399 and name CB)	3.71	0.03	0.02
	assign (segid 3A4 and resid 398 and name C)	(segid 3A4 and resid 399 and name N)	1.33	0.01	0.00
	assign (segid 3A4 and resid 398 and name C)	(segid 3A4 and resid 399 and name O)	3.78	0.11	0.10
	assign (segid 3A4 and resid 398 and name C)	(segid 3A4 and resid 400 and name C)	4.61	0.09	0.09
	assign (segid 3A4 and resid 398 and name C)	(segid 3A4 and resid 400 and name CA)	4.58	0.11	0.10
65	assign (segid 3A4 and resid 398 and name C)	(segid 3A4 and resid 400 and name CB)	5.33	0.14	0.13
	assign (segid 3A4 and resid 398 and name C)	(segid 3A4 and resid 400 and name N)	3.43	0.11	0.11
	assign (segid 3A4 and resid 398 and name C)	(segid 3A4 and resid 400 and name O)	5.65	0.11	0.12
	assign (segid 3A4 and resid 398 and name C)	(segid 3A4 and resid 401 and name C)	4.89	0.08	0.07
	assign (segid 3A4 and resid 398 and name C)	(segid 3A4 and resid 401 and name CA)	4.63	0.07	0.07
70	assign (segid 3A4 and resid 398 and name C)	(segid 3A4 and resid 401 and name N)	3.92	0.07	0.06
	assign (segid 3A4 and resid 398 and name C)	(segid 3A4 and resid 401 and name O)	6.10	0.07	0.08
	assign (segid 3A4 and resid 398 and name C)	(segid 3A4 and resid 402 and name C)	6.00	0.06	0.06
	assign (segid 3A4 and resid 398 and name C)	(segid 3A4 and resid 402 and name CA)	4.98	0.10	0.10
	assign (segid 3A4 and resid 398 and name C)	(segid 3A4 and resid 402 and name CB)	4.50	0.12	0.12
75	assign (segid 3A4 and resid 398 and name C)	(segid 3A4 and resid 402 and name N)	4.11	0.07	0.08
	assign (segid 3A4 and resid 398 and name C)	(segid 3A4 and resid 402 and name O)	7.18	0.08	0.08
	assign (segid 3A4 and resid 398 and name C)	(segid 3A4 and resid 403 and name CA)	7.09	0.06	0.05
	assign (segid 3A4 and resid 398 and name C)	(segid 3A4 and resid 403 and name CB)	7.08	0.08	0.07
	assign (segid 3A4 and resid 398 and name C)	(segid 3A4 and resid 403 and name N)	5.83	0.05	0.04
80	assign (segid 3A4 and resid 398 and name C)	(segid 3A4 and resid 404 and name N)	7.74	0.07	0.06
	assign (segid 3A4 and resid 398 and name CA)	(segid 3A4 and resid 398 and name C)	1.52	0.01	0.01
	assign (segid 3A4 and resid 398 and name CA)	(segid 3A4 and resid 398 and name CB)	1.51	0.02	0.02
	assign (segid 3A4 and resid 398 and name CA)	(segid 3A4 and resid 398 and name CD1)	3.84	0.05	0.05

	assign (segid 3A4 and resid 398 and name CA) (segid 3A4 and resid 398 and name CG)	2.55	0.02	0.02
	assign (segid 3A4 and resid 398 and name CA) (segid 3A4 and resid 398 and name O)	2.38	0.02	0.02
	assign (segid 3A4 and resid 398 and name CA) (segid 3A4 and resid 399 and name C)	4.41	0.05	0.04
	assign (segid 3A4 and resid 398 and name CA) (segid 3A4 and resid 399 and name CA)	3.81	0.01	0.02
5	assign (segid 3A4 and resid 398 and name CA) (segid 3A4 and resid 399 and name CB)	4.86	0.03	0.04
	assign (segid 3A4 and resid 398 and name CA) (segid 3A4 and resid 399 and name N)	2.44	0.02	0.01
	assign (segid 3A4 and resid 398 and name CA) (segid 3A4 and resid 399 and name O)	5.21	0.12	0.12
	assign (segid 3A4 and resid 398 and name CA) (segid 3A4 and resid 400 and name C)	5.52	0.10	0.11
	assign (segid 3A4 and resid 398 and name CA) (segid 3A4 and resid 400 and name CA)	5.54	0.12	0.11
10	assign (segid 3A4 and resid 398 and name CA) (segid 3A4 and resid 400 and name CB)	5.97	0.17	0.18
	assign (segid 3A4 and resid 398 and name CA) (segid 3A4 and resid 400 and name N)	4.50	0.11	0.12
	assign (segid 3A4 and resid 398 and name CA) (segid 3A4 and resid 400 and name O)	6.63	0.13	0.12
	assign (segid 3A4 and resid 398 and name CA) (segid 3A4 and resid 401 and name C)	5.67	0.13	0.12
	assign (segid 3A4 and resid 398 and name CA) (segid 3A4 and resid 401 and name CA)	5.16	0.09	0.09
15	assign (segid 3A4 and resid 398 and name CA) (segid 3A4 and resid 401 and name N)	4.60	0.07	0.08
	assign (segid 3A4 and resid 398 and name CA) (segid 3A4 and resid 401 and name O)	6.87	0.14	0.13
	assign (segid 3A4 and resid 398 and name CA) (segid 3A4 and resid 402 and name C)	7.22	0.10	0.10
	assign (segid 3A4 and resid 398 and name CA) (segid 3A4 and resid 402 and name CA)	6.05	0.13	0.12
	assign (segid 3A4 and resid 398 and name CA) (segid 3A4 and resid 402 and name CB)	5.63	0.13	0.14
20	assign (segid 3A4 and resid 398 and name CA) (segid 3A4 and resid 402 and name N)	5.08	0.11	0.12
	assign (segid 3A4 and resid 398 and name CA) (segid 3A4 and resid 403 and name CA)	8.46	0.07	0.08
	assign (segid 3A4 and resid 398 and name CA) (segid 3A4 and resid 403 and name CB)	8.50	0.09	0.10
	assign (segid 3A4 and resid 398 and name CA) (segid 3A4 and resid 403 and name N)	7.16	0.07	0.07
	assign (segid 3A4 and resid 398 and name CA) (segid 3A4 and resid 404 and name CA)	9.90	0.10	0.09
25	assign (segid 3A4 and resid 398 and name CA) (segid 3A4 and resid 404 and name CB)	9.53	0.11	0.12
	assign (segid 3A4 and resid 398 and name CA) (segid 3A4 and resid 405 and name CA)	10.57	0.15	0.14
	assign (segid 3A4 and resid 398 and name CA) (segid 3A4 and resid 405 and name CB)	9.87	0.13	0.13
	assign (segid 3A4 and resid 398 and name CA) (segid 3A4 and resid 406 and name CA)	11.95	0.15	0.15
	assign (segid 3A4 and resid 398 and name CA) (segid 3A4 and resid 407 and name CA)	14.10	0.08	0.07
30	assign (segid 3A4 and resid 398 and name CA) (segid 3A4 and resid 407 and name CB)	13.86	0.11	0.10
	assign (segid 3A4 and resid 398 and name CA) (segid 3A4 and resid 408 and name CA)	15.30	0.14	0.15
	assign (segid 3A4 and resid 398 and name CA) (segid 3A4 and resid 408 and name CB)	14.71	0.24	0.23
	assign (segid 3A4 and resid 398 and name CA) (segid 3A4 and resid 409 and name CA)	16.61	0.41	0.41
	assign (segid 3A4 and resid 398 and name CA) (segid 3A4 and resid 409 and name CB)	16.00	0.59	0.59
35	assign (segid 3A4 and resid 398 and name CA) (segid 3A4 and resid 410 and name CA)	18.22	0.41	0.40
	assign (segid 3A4 and resid 398 and name CA) (segid 3A4 and resid 433 and name CA)	17.98	0.38	0.39
	assign (segid 3A4 and resid 398 and name CA) (segid 3A4 and resid 434 and name CA)	17.50	0.60	0.60
	assign (segid 3A4 and resid 398 and name CA) (segid 3A4 and resid 435 and name CA)	18.97	0.40	0.40
	assign (segid 3A4 and resid 398 and name CA) (segid HEM and resid 1 and name CAB)	7.43	0.25	0.24
40	assign (segid 3A4 and resid 398 and name CA) (segid HEM and resid 1 and name CBB)	7.16	0.25	0.25
	assign (segid 3A4 and resid 398 and name CA) (segid 3A4 and resid 398 and name CD1)	2.48	0.06	0.05
	assign (segid 3A4 and resid 398 and name CB) (segid 3A4 and resid 398 and name CG)	1.54	0.02	0.01
	assign (segid 3A4 and resid 398 and name CB) (segid 3A4 and resid 399 and name C)	5.46	0.02	0.03
	assign (segid 3A4 and resid 398 and name CB) (segid 3A4 and resid 399 and name CA)	4.54	0.02	0.01
45	assign (segid 3A4 and resid 398 and name CB) (segid 3A4 and resid 399 and name CB)	5.42	0.04	0.04
	assign (segid 3A4 and resid 398 and name CB) (segid 3A4 and resid 399 and name N)	3.22	0.02	0.02
	assign (segid 3A4 and resid 398 and name CB) (segid 3A4 and resid 399 and name O)	6.22	0.09	0.09
	assign (segid 3A4 and resid 398 and name CB) (segid 3A4 and resid 400 and name C)	6.92	0.10	0.10
	assign (segid 3A4 and resid 398 and name CB) (segid 3A4 and resid 400 and name CA)	6.91	0.11	0.10
50	assign (segid 3A4 and resid 398 and name CB) (segid 3A4 and resid 400 and name CB)	7.41	0.16	0.15
	assign (segid 3A4 and resid 398 and name CB) (segid 3A4 and resid 400 and name N)	5.76	0.09	0.09
	assign (segid 3A4 and resid 398 and name CB) (segid 3A4 and resid 401 and name C)	6.78	0.15	0.16
	assign (segid 3A4 and resid 398 and name CB) (segid 3A4 and resid 401 and name CA)	6.47	0.12	0.12
	assign (segid 3A4 and resid 398 and name CB) (segid 3A4 and resid 401 and name N)	6.02	0.08	0.08
55	assign (segid 3A4 and resid 398 and name CB) (segid 3A4 and resid 402 and name CA)	6.77	0.16	0.15
	assign (segid 3A4 and resid 398 and name CB) (segid 3A4 and resid 402 and name CB)	6.07	0.15	0.16
	assign (segid 3A4 and resid 398 and name CB) (segid 3A4 and resid 402 and name N)	6.04	0.13	0.14
	assign (segid 3A4 and resid 398 and name CB) (segid 3A4 and resid 403 and name CA)	9.40	0.06	0.06
	assign (segid 3A4 and resid 398 and name CB) (segid 3A4 and resid 403 and name CB)	9.48	0.07	0.06
60	assign (segid 3A4 and resid 398 and name CB) (segid 3A4 and resid 404 and name CA)	11.12	0.12	0.11
	assign (segid 3A4 and resid 398 and name CB) (segid 3A4 and resid 404 and name CB)	10.85	0.14	0.14
	assign (segid 3A4 and resid 398 and name CB) (segid 3A4 and resid 405 and name CA)	11.53	0.20	0.20
	assign (segid 3A4 and resid 398 and name CB) (segid 3A4 and resid 405 and name CB)	10.73	0.19	0.20
	assign (segid 3A4 and resid 398 and name CB) (segid 3A4 and resid 406 and name CA)	12.66	0.13	0.12
65	assign (segid 3A4 and resid 398 and name CB) (segid 3A4 and resid 407 and name CA)	15.04	0.08	0.09
	assign (segid 3A4 and resid 398 and name CB) (segid 3A4 and resid 407 and name CB)	14.87	0.12	0.13
	assign (segid 3A4 and resid 398 and name CB) (segid 3A4 and resid 408 and name CA)	16.37	0.18	0.19
	assign (segid 3A4 and resid 398 and name CB) (segid 3A4 and resid 408 and name CB)	15.82	0.28	0.29
	assign (segid 3A4 and resid 398 and name CB) (segid 3A4 and resid 409 and name CA)	17.45	0.45	0.45
70	assign (segid 3A4 and resid 398 and name CB) (segid 3A4 and resid 409 and name CB)	16.76	0.63	0.62
	assign (segid 3A4 and resid 398 and name CB) (segid 3A4 and resid 410 and name CA)	18.98	0.40	0.40
	assign (segid 3A4 and resid 398 and name CB) (segid 3A4 and resid 433 and name CA)	18.73	0.43	0.42
	assign (segid 3A4 and resid 398 and name CD1) (segid 3A4 and resid 399 and name C)	7.91	0.05	0.06
75	assign (segid 3A4 and resid 398 and name CD1) (segid 3A4 and resid 399 and name CA)	6.89	0.09	0.08
	assign (segid 3A4 and resid 398 and name CD1) (segid 3A4 and resid 399 and name CB)	7.61	0.12	0.12
	assign (segid 3A4 and resid 398 and name CD1) (segid 3A4 and resid 399 and name N)	5.62	0.09	0.08
	assign (segid 3A4 and resid 398 and name CG) (segid 3A4 and resid 398 and name CD1)	1.52	0.01	0.01
	assign (segid 3A4 and resid 398 and name CG) (segid 3A4 and resid 399 and name C)	6.86	0.03	0.04
80	assign (segid 3A4 and resid 398 and name CG) (segid 3A4 and resid 399 and name CA)	6.03	0.03	0.03
	assign (segid 3A4 and resid 398 and name CG) (segid 3A4 and resid 399 and name CB)	6.90	0.05	0.06
	assign (segid 3A4 and resid 398 and name CG) (segid 3A4 and resid 399 and name N)	4.68	0.04	0.03
	assign (segid 3A4 and resid 398 and name CG) (segid 3A4 and resid 399 and name O)	7.61	0.12	0.12
	assign (segid 3A4 and resid 398 and name CG) (segid 3A4 and resid 400 and name N)	7.04	0.11	0.11

	assign (segid 3A4 and resid 398 and name CG)	(segid 3A4 and resid 401 and name C)	7.63	0.15	0.15
	assign (segid 3A4 and resid 398 and name CG)	(segid 3A4 and resid 401 and name CA)	7.21	0.13	0.13
	assign (segid 3A4 and resid 398 and name CG)	(segid 3A4 and resid 401 and name N)	6.94	0.10	0.09
	assign (segid 3A4 and resid 398 and name CG)	(segid 3A4 and resid 402 and name CB)	7.18	0.10	0.11
	assign (segid 3A4 and resid 398 and name CG)	(segid 3A4 and resid 402 and name N)	7.03	0.12	0.11
5	assign (segid 3A4 and resid 398 and name CG)	(segid HEM and resid 1 and name CAB)	7.60	0.28	0.28
	assign (segid 3A4 and resid 398 and name CG)	(segid HEM and resid 1 and name CBB)	7.34	0.41	0.41
	assign (segid 3A4 and resid 398 and name CG)	(segid HEM and resid 1 and name C)	2.45	0.02	0.02
	assign (segid 3A4 and resid 398 and name N)	(segid 3A4 and resid 398 and name CA)	1.45	0.00	0.01
	assign (segid 3A4 and resid 398 and name N)	(segid 3A4 and resid 398 and name CB)	2.44	0.03	0.03
10	assign (segid 3A4 and resid 398 and name N)	(segid 3A4 and resid 398 and name CD1)	4.39	0.08	0.07
	assign (segid 3A4 and resid 398 and name N)	(segid 3A4 and resid 398 and name CG)	3.12	0.06	0.06
	assign (segid 3A4 and resid 398 and name N)	(segid 3A4 and resid 398 and name O)	3.52	0.03	0.02
	assign (segid 3A4 and resid 398 and name N)	(segid 3A4 and resid 399 and name C)	4.70	0.05	0.06
	assign (segid 3A4 and resid 398 and name N)	(segid 3A4 and resid 399 and name CA)	4.20	0.03	0.03
15	assign (segid 3A4 and resid 398 and name N)	(segid 3A4 and resid 399 and name CB)	4.94	0.06	0.06
	assign (segid 3A4 and resid 398 and name N)	(segid 3A4 and resid 399 and name N)	2.78	0.03	0.04
	assign (segid 3A4 and resid 398 and name N)	(segid 3A4 and resid 399 and name O)	5.71	0.12	0.12
	assign (segid 3A4 and resid 398 and name N)	(segid 3A4 and resid 400 and name C)	5.67	0.08	0.08
	assign (segid 3A4 and resid 398 and name N)	(segid 3A4 and resid 400 and name CA)	5.42	0.11	0.12
20	assign (segid 3A4 and resid 398 and name N)	(segid 3A4 and resid 400 and name CB)	5.51	0.19	0.19
	assign (segid 3A4 and resid 398 and name N)	(segid 3A4 and resid 400 and name N)	4.44	0.10	0.09
	assign (segid 3A4 and resid 398 and name N)	(segid 3A4 and resid 400 and name O)	6.86	0.09	0.09
	assign (segid 3A4 and resid 398 and name N)	(segid 3A4 and resid 401 and name C)	6.43	0.10	0.11
	assign (segid 3A4 and resid 398 and name N)	(segid 3A4 and resid 401 and name CA)	5.64	0.07	0.08
25	assign (segid 3A4 and resid 398 and name N)	(segid 3A4 and resid 401 and name N)	4.86	0.06	0.07
	assign (segid 3A4 and resid 398 and name N)	(segid 3A4 and resid 401 and name O)	7.64	0.10	0.11
	assign (segid 3A4 and resid 398 and name N)	(segid 3A4 and resid 402 and name CA)	7.14	0.10	0.10
	assign (segid 3A4 and resid 398 and name N)	(segid 3A4 and resid 402 and name CB)	6.86	0.12	0.11
	assign (segid 3A4 and resid 398 and name N)	(segid 3A4 and resid 402 and name N)	6.03	0.09	0.09
30	assign (segid 3A4 and resid 398 and name N)	(segid HEM and resid 1 and name C3B)	7.26	0.21	0.20
	assign (segid 3A4 and resid 398 and name N)	(segid HEM and resid 1 and name C4B)	7.52	0.20	0.20
	assign (segid 3A4 and resid 398 and name N)	(segid HEM and resid 1 and name CAB)	6.47	0.21	0.22
	assign (segid 3A4 and resid 398 and name N)	(segid HEM and resid 1 and name CBB)	6.42	0.23	0.22
	assign (segid 3A4 and resid 398 and name N)	(segid HEM and resid 1 and name CHC)	7.12	0.21	0.21
35	assign (segid 3A4 and resid 398 and name N)	(segid HEM and resid 1 and name CMC)	7.03	0.32	0.32
	assign (segid 3A4 and resid 398 and name N)	(segid 3A4 and resid 398 and name CB)	3.21	0.04	0.04
	assign (segid 3A4 and resid 398 and name O)	(segid 3A4 and resid 398 and name CD1)	5.52	0.09	0.10
	assign (segid 3A4 and resid 398 and name O)	(segid 3A4 and resid 398 and name CG)	4.45	0.05	0.06
	assign (segid 3A4 and resid 398 and name O)	(segid 3A4 and resid 399 and name C)	3.03	0.05	0.05
40	assign (segid 3A4 and resid 398 and name O)	(segid 3A4 and resid 399 and name CA)	2.77	0.03	0.02
	assign (segid 3A4 and resid 398 and name O)	(segid 3A4 and resid 399 and name CB)	4.24	0.04	0.04
	assign (segid 3A4 and resid 398 and name O)	(segid 3A4 and resid 399 and name N)	2.24	0.01	0.02
	assign (segid 3A4 and resid 398 and name O)	(segid 3A4 and resid 399 and name O)	3.37	0.12	0.11
	assign (segid 3A4 and resid 398 and name O)	(segid 3A4 and resid 400 and name C)	4.27	0.16	0.17
45	assign (segid 3A4 and resid 398 and name O)	(segid 3A4 and resid 400 and name CA)	4.57	0.17	0.17
	assign (segid 3A4 and resid 398 and name O)	(segid 3A4 and resid 400 and name CB)	5.56	0.16	0.16
	assign (segid 3A4 and resid 398 and name O)	(segid 3A4 and resid 400 and name N)	3.64	0.15	0.16
	assign (segid 3A4 and resid 398 and name O)	(segid 3A4 and resid 400 and name O)	5.14	0.18	0.18
	assign (segid 3A4 and resid 398 and name O)	(segid 3A4 and resid 401 and name C)	3.93	0.14	0.14
50	assign (segid 3A4 and resid 398 and name O)	(segid 3A4 and resid 401 and name CA)	3.97	0.14	0.15
	assign (segid 3A4 and resid 398 and name O)	(segid 3A4 and resid 401 and name N)	3.53	0.15	0.15
	assign (segid 3A4 and resid 398 and name O)	(segid 3A4 and resid 401 and name O)	5.10	0.13	0.13
	assign (segid 3A4 and resid 398 and name O)	(segid 3A4 and resid 402 and name C)	4.90	0.10	0.10
	assign (segid 3A4 and resid 398 and name O)	(segid 3A4 and resid 402 and name CA)	3.79	0.11	0.12
55	assign (segid 3A4 and resid 398 and name O)	(segid 3A4 and resid 402 and name CB)	3.35	0.12	0.12
	assign (segid 3A4 and resid 398 and name O)	(segid 3A4 and resid 402 and name N)	3.01	0.12	0.12
	assign (segid 3A4 and resid 398 and name O)	(segid 3A4 and resid 402 and name O)	6.04	0.11	0.11
	assign (segid 3A4 and resid 398 and name O)	(segid 3A4 and resid 403 and name C)	7.15	0.10	0.11
	assign (segid 3A4 and resid 398 and name O)	(segid 3A4 and resid 403 and name CA)	6.24	0.10	0.09
60	assign (segid 3A4 and resid 398 and name O)	(segid 3A4 and resid 403 and name CB)	6.45	0.10	0.10
	assign (segid 3A4 and resid 398 and name O)	(segid 3A4 and resid 403 and name N)	4.89	0.09	0.09
	assign (segid 3A4 and resid 398 and name O)	(segid 3A4 and resid 404 and name N)	6.91	0.16	0.16
	assign (segid 3A4 and resid 399 and name C)	(segid 3A4 and resid 399 and name CB)	2.50	0.02	0.02
65	assign (segid 3A4 and resid 399 and name C)	(segid 3A4 and resid 399 and name O)	1.24	0.02	0.01
	assign (segid 3A4 and resid 399 and name C)	(segid 3A4 and resid 400 and name C)	3.00	0.07	0.06
	assign (segid 3A4 and resid 399 and name C)	(segid 3A4 and resid 400 and name CA)	2.43	0.01	0.01
	assign (segid 3A4 and resid 399 and name C)	(segid 3A4 and resid 400 and name CB)	3.68	0.05	0.04
	assign (segid 3A4 and resid 399 and name C)	(segid 3A4 and resid 400 and name N)	1.32	0.01	0.02
70	assign (segid 3A4 and resid 399 and name C)	(segid 3A4 and resid 400 and name O)	3.82	0.09	0.10
	assign (segid 3A4 and resid 399 and name C)	(segid 3A4 and resid 401 and name C)	4.56	0.12	0.12
	assign (segid 3A4 and resid 399 and name C)	(segid 3A4 and resid 401 and name CA)	4.47	0.13	0.14
	assign (segid 3A4 and resid 399 and name C)	(segid 3A4 and resid 401 and name N)	3.30	0.13	0.13
	assign (segid 3A4 and resid 399 and name C)	(segid 3A4 and resid 401 and name O)	5.60	0.14	0.14
	assign (segid 3A4 and resid 399 and name C)	(segid 3A4 and resid 402 and name C)	4.90	0.10	0.09
75	assign (segid 3A4 and resid 399 and name C)	(segid 3A4 and resid 402 and name CA)	4.66	0.10	0.10
	assign (segid 3A4 and resid 399 and name C)	(segid 3A4 and resid 402 and name CB)	4.54	0.12	0.11
	assign (segid 3A4 and resid 399 and name C)	(segid 3A4 and resid 402 and name N)	3.91	0.10	0.11
	assign (segid 3A4 and resid 399 and name C)	(segid 3A4 and resid 402 and name O)	6.10	0.10	0.11
	assign (segid 3A4 and resid 399 and name C)	(segid 3A4 and resid 403 and name C)	5.26	0.14	0.14
80	assign (segid 3A4 and resid 399 and name C)	(segid 3A4 and resid 403 and name CA)	4.94	0.08	0.08
	assign (segid 3A4 and resid 399 and name C)	(segid 3A4 and resid 403 and name CB)	4.46	0.06	0.06
	assign (segid 3A4 and resid 399 and name C)	(segid 3A4 and resid 403 and name N)	4.09	0.09	0.10

assign (segid 3A4 and resid 399 and name C) (segid 3A4 and resid 403 and name O) 7.13 0.13 0.13
 assign (segid 3A4 and resid 399 and name C) (segid 3A4 and resid 404 and name CA) 7.02 0.20 0.20
 assign (segid 3A4 and resid 399 and name C) (segid 3A4 and resid 404 and name CB) 7.02 0.23 0.22
 assign (segid 3A4 and resid 399 and name C) (segid 3A4 and resid 404 and name N) 5.77 0.19 0.19
 5 assign (segid 3A4 and resid 399 and name C) (segid 3A4 and resid 405 and name N) 7.71 0.20 0.19
 assign (segid 3A4 and resid 399 and name CA) (segid 3A4 and resid 399 and name C) 1.53 0.01 0.00
 assign (segid 3A4 and resid 399 and name CA) (segid 3A4 and resid 399 and name CB) 1.52 0.01 0.02
 assign (segid 3A4 and resid 399 and name CA) (segid 3A4 and resid 399 and name O) 2.40 0.02 0.02
 assign (segid 3A4 and resid 399 and name CA) (segid 3A4 and resid 400 and name C) 4.40 0.04 0.04
 10 assign (segid 3A4 and resid 399 and name CA) (segid 3A4 and resid 400 and name CB) 3.81 0.01 0.02
 assign (segid 3A4 and resid 399 and name CA) (segid 3A4 and resid 400 and name N) 2.45 0.02 0.06
 assign (segid 3A4 and resid 399 and name CA) (segid 3A4 and resid 400 and name O) 5.29 0.09 0.09
 assign (segid 3A4 and resid 399 and name CA) (segid 3A4 and resid 401 and name C) 5.52 0.08 0.08
 15 assign (segid 3A4 and resid 399 and name CA) (segid 3A4 and resid 401 and name N) 5.49 0.09 0.09
 assign (segid 3A4 and resid 399 and name CA) (segid 3A4 and resid 401 and name O) 4.42 0.09 0.08
 assign (segid 3A4 and resid 399 and name CA) (segid 3A4 and resid 402 and name C) 6.63 0.09 0.09
 assign (segid 3A4 and resid 399 and name CA) (segid 3A4 and resid 402 and name CB) 5.69 0.08 0.07
 assign (segid 3A4 and resid 399 and name CA) (segid 3A4 and resid 402 and name CA) 5.22 0.06 0.07
 20 assign (segid 3A4 and resid 399 and name CA) (segid 3A4 and resid 402 and name N) 4.66 0.10 0.09
 assign (segid 3A4 and resid 399 and name CA) (segid 3A4 and resid 402 and name O) 4.64 0.06 0.07
 assign (segid 3A4 and resid 399 and name CA) (segid 3A4 and resid 403 and name C) 7.17 0.15 0.14
 assign (segid 3A4 and resid 399 and name CA) (segid 3A4 and resid 403 and name CB) 5.99 0.11 0.11
 25 assign (segid 3A4 and resid 399 and name CA) (segid 3A4 and resid 403 and name N) 5.55 0.12 0.13
 assign (segid 3A4 and resid 399 and name CA) (segid 3A4 and resid 404 and name C) 5.06 0.10 0.10
 assign (segid 3A4 and resid 399 and name CA) (segid 3A4 and resid 404 and name CB) 8.41 0.17 0.17
 assign (segid 3A4 and resid 399 and name CA) (segid 3A4 and resid 404 and name N) 8.46 0.19 0.18
 30 assign (segid 3A4 and resid 399 and name CA) (segid 3A4 and resid 405 and name CA) 7.11 0.17 0.17
 assign (segid 3A4 and resid 399 and name CA) (segid 3A4 and resid 405 and name CB) 9.97 0.14 0.14
 assign (segid 3A4 and resid 399 and name CA) (segid 3A4 and resid 406 and name CA) 9.75 0.20 0.20
 assign (segid 3A4 and resid 399 and name CA) (segid 3A4 and resid 407 and name CA) 10.49 0.13 0.13
 assign (segid 3A4 and resid 399 and name CA) (segid 3A4 and resid 407 and name CB) 12.08 0.20 0.20
 35 assign (segid 3A4 and resid 399 and name CA) (segid 3A4 and resid 408 and name CA) 11.60 0.23 0.23
 assign (segid 3A4 and resid 399 and name CA) (segid 3A4 and resid 408 and name CB) 14.04 0.12 0.11
 assign (segid 3A4 and resid 399 and name CA) (segid 3A4 and resid 409 and name CA) 13.76 0.08 0.08
 assign (segid 3A4 and resid 399 and name CA) (segid 3A4 and resid 409 and name CB) 15.70 0.40 0.40
 assign (segid 3A4 and resid 399 and name CA) (segid 3A4 and resid 409 and name N) 15.32 0.59 0.60
 40 assign (segid 3A4 and resid 399 and name CA) (segid 3A4 and resid 410 and name CA) 16.63 0.52 0.53
 assign (segid 3A4 and resid 399 and name CA) (segid 3A4 and resid 411 and name CA) 18.33 0.36 0.36
 assign (segid 3A4 and resid 399 and name CA) (segid 3A4 and resid 411 and name CB) 17.75 0.40 0.40
 assign (segid 3A4 and resid 399 and name CB) (segid 3A4 and resid 400 and name C) 5.39 0.08 0.08
 45 assign (segid 3A4 and resid 399 and name CB) (segid 3A4 and resid 400 and name CA) 4.44 0.07 0.06
 assign (segid 3A4 and resid 399 and name CB) (segid 3A4 and resid 400 and name CB) 5.27 0.10 0.10
 assign (segid 3A4 and resid 399 and name CB) (segid 3A4 and resid 400 and name N) 3.10 0.08 0.08
 assign (segid 3A4 and resid 399 and name CB) (segid 3A4 and resid 401 and name O) 6.24 0.10 0.11
 assign (segid 3A4 and resid 399 and name CB) (segid 3A4 and resid 401 and name CA) 6.92 0.11 0.10
 50 assign (segid 3A4 and resid 399 and name CB) (segid 3A4 and resid 401 and name N) 6.82 0.09 0.09
 assign (segid 3A4 and resid 399 and name CB) (segid 3A4 and resid 402 and name C) 5.62 0.10 0.09
 assign (segid 3A4 and resid 399 and name CB) (segid 3A4 and resid 402 and name CB) 6.88 0.13 0.12
 assign (segid 3A4 and resid 399 and name CB) (segid 3A4 and resid 402 and name CA) 6.59 0.08 0.09
 55 assign (segid 3A4 and resid 399 and name CB) (segid 3A4 and resid 402 and name N) 5.97 0.09 0.09
 assign (segid 3A4 and resid 399 and name CB) (segid 3A4 and resid 402 and name O) 6.09 0.08 0.07
 assign (segid 3A4 and resid 399 and name CB) (segid 3A4 and resid 403 and name CA) 6.77 0.19 0.19
 assign (segid 3A4 and resid 399 and name CB) (segid 3A4 and resid 403 and name CB) 6.04 0.22 0.22
 60 assign (segid 3A4 and resid 399 and name CB) (segid 3A4 and resid 403 and name N) 6.08 0.16 0.17
 assign (segid 3A4 and resid 399 and name CB) (segid 3A4 and resid 404 and name CA) 9.33 0.28 0.29
 assign (segid 3A4 and resid 399 and name CB) (segid 3A4 and resid 404 and name CB) 9.41 0.30 0.29
 assign (segid 3A4 and resid 399 and name CB) (segid 3A4 and resid 405 and name CA) 11.22 0.20 0.19
 assign (segid 3A4 and resid 399 and name CB) (segid 3A4 and resid 405 and name CB) 11.10 0.24 0.25
 65 assign (segid 3A4 and resid 399 and name CB) (segid 3A4 and resid 406 and name CA) 11.54 0.17 0.16
 assign (segid 3A4 and resid 399 and name CB) (segid 3A4 and resid 407 and name CA) 12.87 0.29 0.28
 assign (segid 3A4 and resid 399 and name CB) (segid 3A4 and resid 407 and name CB) 12.26 0.34 0.33
 assign (segid 3A4 and resid 399 and name CB) (segid 3A4 and resid 408 and name CA) 15.01 0.22 0.21
 70 assign (segid 3A4 and resid 399 and name CB) (segid 3A4 and resid 408 and name CB) 14.80 0.15 0.16
 assign (segid 3A4 and resid 399 and name CB) (segid 3A4 and resid 409 and name CA) 16.82 0.43 0.43
 assign (segid 3A4 and resid 399 and name CB) (segid 3A4 and resid 409 and name CB) 16.51 0.62 0.62
 assign (segid 3A4 and resid 399 and name CB) (segid 3A4 and resid 410 and name CA) 17.54 0.59 0.60
 75 assign (segid 3A4 and resid 399 and name CB) (segid 3A4 and resid 411 and name CB) 18.50 0.47 0.48
 assign (segid 3A4 and resid 399 and name N) (segid 3A4 and resid 399 and name C) 2.44 0.03 0.04
 assign (segid 3A4 and resid 399 and name N) (segid 3A4 and resid 399 and name CA) 1.46 0.01 0.01
 assign (segid 3A4 and resid 399 and name N) (segid 3A4 and resid 399 and name CB) 2.45 0.04 0.04
 assign (segid 3A4 and resid 399 and name N) (segid 3A4 and resid 399 and name O) 3.44 0.06 0.06
 80 assign (segid 3A4 and resid 399 and name N) (segid 3A4 and resid 400 and name C) 4.69 0.02 0.01
 assign (segid 3A4 and resid 399 and name N) (segid 3A4 and resid 400 and name CA) 4.23 0.04 0.04
 assign (segid 3A4 and resid 399 and name N) (segid 3A4 and resid 400 and name N) 2.86 0.04 0.04
 assign (segid 3A4 and resid 399 and name N) (segid 3A4 and resid 401 and name N) 5.75 0.07 0.08
 assign (segid 3A4 and resid 399 and name N) (segid 3A4 and resid 401 and name C) 5.61 0.02 0.02
 assign (segid 3A4 and resid 399 and name N) (segid 3A4 and resid 401 and name CA) 5.33 0.04 0.05
 assign (segid 3A4 and resid 399 and name N) (segid 3A4 and resid 401 and name N) 4.33 0.05 0.04
 assign (segid 3A4 and resid 399 and name N) (segid 3A4 and resid 401 and name O) 6.81 0.03 0.03
 assign (segid 3A4 and resid 399 and name N) (segid 3A4 and resid 402 and name C) 6.39 0.04 0.03

	assign (segid 3A4 and resid 399 and name N)	(segid 3A4 and resid 402 and name CA)	5.62	0.07	0.06
	assign (segid 3A4 and resid 399 and name N)	(segid 3A4 and resid 402 and name CB)	5.07	0.11	0.10
	assign (segid 3A4 and resid 399 and name N)	(segid 3A4 and resid 402 and name N)	4.82	0.03	0.03
	assign (segid 3A4 and resid 399 and name N)	(segid 3A4 and resid 402 and name O)	7.59	0.05	0.05
5	assign (segid 3A4 and resid 399 and name N)	(segid 3A4 and resid 403 and name CA)	7.05	0.07	0.08
	assign (segid 3A4 and resid 399 and name N)	(segid 3A4 and resid 403 and name CB)	6.76	0.09	0.10
	assign (segid 3A4 and resid 399 and name N)	(segid 3A4 and resid 403 and name N)	5.96	0.05	0.05
	assign (segid 3A4 and resid 399 and name N)	(segid 3A4 and resid 399 and name CB)	3.36	0.07	0.07
	assign (segid 3A4 and resid 399 and name O)	(segid 3A4 and resid 400 and name C)	2.91	0.13	0.13
10	assign (segid 3A4 and resid 399 and name O)	(segid 3A4 and resid 400 and name CA)	2.74	0.03	0.04
	assign (segid 3A4 and resid 399 and name O)	(segid 3A4 and resid 400 and name CB)	4.21	0.05	0.05
	assign (segid 3A4 and resid 399 and name O)	(segid 3A4 and resid 400 and name N)	2.23	0.02	0.03
	assign (segid 3A4 and resid 399 and name O)	(segid 3A4 and resid 400 and name O)	3.37	0.15	0.16
	assign (segid 3A4 and resid 399 and name O)	(segid 3A4 and resid 401 and name C)	4.03	0.27	0.28
15	assign (segid 3A4 and resid 399 and name O)	(segid 3A4 and resid 401 and name CA)	4.30	0.28	0.27
	assign (segid 3A4 and resid 399 and name O)	(segid 3A4 and resid 401 and name N)	3.37	0.24	0.24
	assign (segid 3A4 and resid 399 and name O)	(segid 3A4 and resid 401 and name O)	4.92	0.27	0.28
	assign (segid 3A4 and resid 399 and name O)	(segid 3A4 and resid 402 and name C)	3.83	0.14	0.15
	assign (segid 3A4 and resid 399 and name O)	(segid 3A4 and resid 402 and name CA)	3.85	0.20	0.20
20	assign (segid 3A4 and resid 399 and name O)	(segid 3A4 and resid 402 and name CB)	3.86	0.15	0.14
	assign (segid 3A4 and resid 399 and name O)	(segid 3A4 and resid 402 and name N)	3.34	0.26	0.25
	assign (segid 3A4 and resid 399 and name O)	(segid 3A4 and resid 402 and name O)	5.00	0.13	0.14
	assign (segid 3A4 and resid 399 and name O)	(segid 3A4 and resid 403 and name C)	4.85	0.10	0.10
	assign (segid 3A4 and resid 399 and name O)	(segid 3A4 and resid 403 and name CA)	3.76	0.03	0.03
25	assign (segid 3A4 and resid 399 and name O)	(segid 3A4 and resid 403 and name CB)	3.41	0.12	0.12
	assign (segid 3A4 and resid 399 and name O)	(segid 3A4 and resid 403 and name N)	2.94	0.10	0.10
	assign (segid 3A4 and resid 399 and name O)	(segid 3A4 and resid 403 and name O)	5.99	0.09	0.10
	assign (segid 3A4 and resid 399 and name O)	(segid 3A4 and resid 404 and name C)	7.03	0.22	0.22
	assign (segid 3A4 and resid 399 and name O)	(segid 3A4 and resid 404 and name CA)	6.14	0.20	0.19
30	assign (segid 3A4 and resid 399 and name O)	(segid 3A4 and resid 404 and name CB)	6.34	0.23	0.23
	assign (segid 3A4 and resid 399 and name O)	(segid 3A4 and resid 404 and name N)	4.80	0.17	0.17
	assign (segid 3A4 and resid 399 and name O)	(segid 3A4 and resid 405 and name N)	6.81	0.23	0.24
	assign (segid 3A4 and resid 399 and name O)	(segid 3A4 and resid 406 and name N)	7.70	0.21	0.21
	assign (segid 3A4 and resid 39 and name C)	(segid 3A4 and resid 345 and name CB)	5.99	0.66	0.66
35	assign (segid 3A4 and resid 39 and name C)	(segid 3A4 and resid 350 and name CB)	6.93	0.54	0.54
	assign (segid 3A4 and resid 39 and name C)	(segid 3A4 and resid 39 and name CB)	2.54	0.04	0.03
	assign (segid 3A4 and resid 39 and name C)	(segid 3A4 and resid 39 and name O)	1.23	0.01	0.01
	assign (segid 3A4 and resid 39 and name C)	(segid 3A4 and resid 40 and name C)	2.99	0.04	0.04
	assign (segid 3A4 and resid 39 and name C)	(segid 3A4 and resid 40 and name CA)	2.43	0.01	0.02
40	assign (segid 3A4 and resid 39 and name C)	(segid 3A4 and resid 40 and name CB)	3.72	0.02	0.02
	assign (segid 3A4 and resid 39 and name C)	(segid 3A4 and resid 40 and name N)	1.32	0.01	0.02
	assign (segid 3A4 and resid 39 and name C)	(segid 3A4 and resid 40 and name O)	3.82	0.09	0.09
	assign (segid 3A4 and resid 39 and name C)	(segid 3A4 and resid 41 and name C)	4.50	0.09	0.10
45	assign (segid 3A4 and resid 39 and name C)	(segid 3A4 and resid 41 and name CB)	5.07	0.09	0.09
	assign (segid 3A4 and resid 39 and name C)	(segid 3A4 and resid 41 and name N)	3.20	0.07	0.08
	assign (segid 3A4 and resid 39 and name C)	(segid 3A4 and resid 41 and name O)	5.58	0.11	0.11
	assign (segid 3A4 and resid 39 and name C)	(segid 3A4 and resid 42 and name C)	4.87	0.08	0.08
	assign (segid 3A4 and resid 39 and name C)	(segid 3A4 and resid 42 and name CA)	4.59	0.11	0.12
50	assign (segid 3A4 and resid 39 and name C)	(segid 3A4 and resid 42 and name CB)	4.46	0.12	0.12
	assign (segid 3A4 and resid 39 and name C)	(segid 3A4 and resid 42 and name N)	3.83	0.11	0.11
	assign (segid 3A4 and resid 39 and name C)	(segid 3A4 and resid 42 and name O)	6.05	0.09	0.10
	assign (segid 3A4 and resid 39 and name CA)	(segid 3A4 and resid 313 and name CA)	17.04	0.54	0.53
55	assign (segid 3A4 and resid 39 and name CA)	(segid 3A4 and resid 313 and name CB)	16.85	0.48	0.48
	assign (segid 3A4 and resid 39 and name CA)	(segid 3A4 and resid 314 and name CA)	14.89	0.54	0.54
	assign (segid 3A4 and resid 39 and name CA)	(segid 3A4 and resid 314 and name CB)	15.16	0.51	0.51
	assign (segid 3A4 and resid 39 and name CA)	(segid 3A4 and resid 315 and name CA)	17.01	0.61	0.61
	assign (segid 3A4 and resid 39 and name CA)	(segid 3A4 and resid 315 and name CB)	18.47	0.59	0.59
	assign (segid 3A4 and resid 39 and name CA)	(segid 3A4 and resid 316 and name CA)	17.47	0.78	0.78
60	assign (segid 3A4 and resid 39 and name CA)	(segid 3A4 and resid 317 and name CA)	14.53	0.70	0.69
	assign (segid 3A4 and resid 39 and name CA)	(segid 3A4 and resid 318 and name CA)	16.41	0.93	0.94
	assign (segid 3A4 and resid 39 and name CA)	(segid 3A4 and resid 318 and name CB)	17.48	0.89	0.90
	assign (segid 3A4 and resid 39 and name CA)	(segid 3A4 and resid 319 and name CA)	14.11	0.99	0.98
	assign (segid 3A4 and resid 39 and name CA)	(segid 3A4 and resid 319 and name CB)	13.86	1.09	1.09
65	assign (segid 3A4 and resid 39 and name CA)	(segid 3A4 and resid 322 and name CA)	11.00	1.00	1.00
	assign (segid 3A4 and resid 39 and name CA)	(segid 3A4 and resid 323 and name CA)	10.98	0.39	0.39
	assign (segid 3A4 and resid 39 and name CA)	(segid 3A4 and resid 323 and name CB)	9.77	0.38	0.39
	assign (segid 3A4 and resid 39 and name CA)	(segid 3A4 and resid 324 and name CA)	13.49	0.31	0.30
	assign (segid 3A4 and resid 39 and name CA)	(segid 3A4 and resid 324 and name CB)	14.93	0.28	0.28
70	assign (segid 3A4 and resid 39 and name CA)	(segid 3A4 and resid 325 and name CA)	13.71	0.36	0.36
	assign (segid 3A4 and resid 39 and name CA)	(segid 3A4 and resid 325 and name CB)	13.67	0.32	0.32
	assign (segid 3A4 and resid 39 and name CA)	(segid 3A4 and resid 326 and name CA)	16.64	0.44	0.44
	assign (segid 3A4 and resid 39 and name CA)	(segid 3A4 and resid 326 and name CB)	16.71	0.50	0.49
	assign (segid 3A4 and resid 39 and name CA)	(segid 3A4 and resid 327 and name CA)	17.68	0.46	0.45
75	assign (segid 3A4 and resid 39 and name CA)	(segid 3A4 and resid 327 and name CB)	17.98	0.50	0.51
	assign (segid 3A4 and resid 39 and name CA)	(segid 3A4 and resid 328 and name CA)	17.21	0.52	0.52
	assign (segid 3A4 and resid 39 and name CA)	(segid 3A4 and resid 328 and name CB)	18.43	0.56	0.57
	assign (segid 3A4 and resid 39 and name CA)	(segid 3A4 and resid 329 and name CA)	14.32	0.69	0.69
	assign (segid 3A4 and resid 39 and name CA)	(segid 3A4 and resid 329 and name CB)	13.19	0.67	0.67
80	assign (segid 3A4 and resid 39 and name CA)	(segid 3A4 and resid 330 and name CA)	13.55	0.87	0.87
	assign (segid 3A4 and resid 39 and name CA)	(segid 3A4 and resid 330 and name CB)	14.71	0.92	0.92
	assign (segid 3A4 and resid 39 and name CA)	(segid 3A4 and resid 331 and name CA)	10.12	0.84	0.84
	assign (segid 3A4 and resid 39 and name CA)	(segid 3A4 and resid 331 and name CB)	9.10	0.82	0.83

	assign (segid 3A4 and resid 39 and name CA) (segid 3A4 and resid 332 and name CA)	10.84	0.95	0.94
	assign (segid 3A4 and resid 39 and name CA) (segid 3A4 and resid 333 and name CA)	14.37	0.84	0.83
	assign (segid 3A4 and resid 39 and name CA) (segid 3A4 and resid 335 and name CA)	13.92	0.72	0.72
	assign (segid 3A4 and resid 39 and name CA) (segid 3A4 and resid 336 and name CA)	15.36	0.59	0.60
5	assign (segid 3A4 and resid 39 and name CA) (segid 3A4 and resid 336 and name CB)	16.86	0.61	0.61
	assign (segid 3A4 and resid 39 and name CA) (segid 3A4 and resid 337 and name CA)	14.23	0.48	0.48
	assign (segid 3A4 and resid 39 and name CA) (segid 3A4 and resid 337 and name CB)	12.86	0.46	0.45
	assign (segid 3A4 and resid 39 and name CA) (segid 3A4 and resid 338 and name CA)	17.32	0.38	0.39
	assign (segid 3A4 and resid 39 and name CA) (segid 3A4 and resid 338 and name CB)	18.44	0.46	0.45
10	assign (segid 3A4 and resid 39 and name CA) (segid 3A4 and resid 339 and name CA)	18.01	0.30	0.30
	assign (segid 3A4 and resid 39 and name CA) (segid 3A4 and resid 339 and name CB)	19.28	0.30	0.30
	assign (segid 3A4 and resid 39 and name CA) (segid 3A4 and resid 340 and name CA)	17.94	0.42	0.41
	assign (segid 3A4 and resid 39 and name CA) (segid 3A4 and resid 340 and name CB)	15.57	0.35	0.35
	assign (segid 3A4 and resid 39 and name CA) (segid 3A4 and resid 341 and name CA)	15.02	0.41	0.41
	assign (segid 3A4 and resid 39 and name CA) (segid 3A4 and resid 341 and name CB)	13.66	0.30	0.30
15	assign (segid 3A4 and resid 39 and name CA) (segid 3A4 and resid 342 and name CA)	10.03	0.22	0.22
	assign (segid 3A4 and resid 39 and name CA) (segid 3A4 and resid 343 and name CA)	9.09	0.34	0.33
	assign (segid 3A4 and resid 39 and name CA) (segid 3A4 and resid 343 and name CB)	9.16	0.23	0.23
	assign (segid 3A4 and resid 39 and name CA) (segid 3A4 and resid 344 and name CA)	10.27	0.30	0.30
20	assign (segid 3A4 and resid 39 and name CA) (segid 3A4 and resid 344 and name CB)	5.96	0.52	0.52
	assign (segid 3A4 and resid 39 and name CA) (segid 3A4 and resid 345 and name CA)	5.29	0.57	0.57
	assign (segid 3A4 and resid 39 and name CA) (segid 3A4 and resid 345 and name CB)	7.16	0.40	0.39
	assign (segid 3A4 and resid 39 and name CA) (segid 3A4 and resid 346 and name CA)	7.60	0.68	0.68
	assign (segid 3A4 and resid 39 and name CA) (segid 3A4 and resid 346 and name CB)	8.26	0.58	0.59
25	assign (segid 3A4 and resid 39 and name CA) (segid 3A4 and resid 347 and name CA)	7.70	0.75	0.76
	assign (segid 3A4 and resid 39 and name CA) (segid 3A4 and resid 347 and name CB)	8.49	0.78	0.79
	assign (segid 3A4 and resid 39 and name CA) (segid 3A4 and resid 348 and name CA)	10.72	0.74	0.74
	assign (segid 3A4 and resid 39 and name CA) (segid 3A4 and resid 349 and name CA)	9.42	0.59	0.59
	assign (segid 3A4 and resid 39 and name CA) (segid 3A4 and resid 349 and name CB)	8.95	0.63	0.63
30	assign (segid 3A4 and resid 39 and name CA) (segid 3A4 and resid 350 and name CA)	7.29	0.46	0.46
	assign (segid 3A4 and resid 39 and name CA) (segid 3A4 and resid 350 and name CB)	6.29	0.58	0.59
	assign (segid 3A4 and resid 39 and name CA) (segid 3A4 and resid 351 and name CA)	10.57	0.51	0.50
	assign (segid 3A4 and resid 39 and name CA) (segid 3A4 and resid 352 and name CA)	12.51	0.45	0.46
	assign (segid 3A4 and resid 39 and name CA) (segid 3A4 and resid 352 and name CB)	13.09	0.50	0.49
35	assign (segid 3A4 and resid 39 and name CA) (segid 3A4 and resid 353 and name CA)	11.15	0.46	0.45
	assign (segid 3A4 and resid 39 and name CA) (segid 3A4 and resid 353 and name CB)	9.87	0.55	0.55
	assign (segid 3A4 and resid 39 and name CA) (segid 3A4 and resid 354 and name CA)	14.53	0.49	0.49
	assign (segid 3A4 and resid 39 and name CA) (segid 3A4 and resid 354 and name CB)	15.47	0.47	0.46
40	assign (segid 3A4 and resid 39 and name CA) (segid 3A4 and resid 355 and name CA)	13.66	0.84	0.84
	assign (segid 3A4 and resid 39 and name CA) (segid 3A4 and resid 355 and name CB)	12.85	0.94	0.93
	assign (segid 3A4 and resid 39 and name CA) (segid 3A4 and resid 356 and name CA)	12.72	0.77	0.76
	assign (segid 3A4 and resid 39 and name CA) (segid 3A4 and resid 356 and name CB)	11.36	0.75	0.75
	assign (segid 3A4 and resid 39 and name CA) (segid 3A4 and resid 357 and name CA)	15.15	0.71	0.71
	assign (segid 3A4 and resid 39 and name CA) (segid 3A4 and resid 357 and name CB)	14.79	0.70	0.70
45	assign (segid 3A4 and resid 39 and name CA) (segid 3A4 and resid 358 and name CA)	18.59	0.68	0.69
	assign (segid 3A4 and resid 39 and name CA) (segid 3A4 and resid 360 and name CA)	17.04	0.58	0.58
	assign (segid 3A4 and resid 39 and name CA) (segid 3A4 and resid 360 and name CB)	15.80	0.63	0.62
	assign (segid 3A4 and resid 39 and name CA) (segid 3A4 and resid 381 and name CA)	11.01	0.49	0.50
	assign (segid 3A4 and resid 39 and name CA) (segid 3A4 and resid 382 and name CA)	8.98	0.54	0.54
50	assign (segid 3A4 and resid 39 and name CA) (segid 3A4 and resid 382 and name CB)	7.49	0.53	0.53
	assign (segid 3A4 and resid 39 and name CA) (segid 3A4 and resid 383 and name CA)	11.83	0.53	0.53
	assign (segid 3A4 and resid 39 and name CA) (segid 3A4 and resid 384 and name CA)	12.79	0.61	0.61
	assign (segid 3A4 and resid 39 and name CA) (segid 3A4 and resid 384 and name CB)	13.83	0.59	0.58
	assign (segid 3A4 and resid 39 and name CA) (segid 3A4 and resid 385 and name CA)	9.62	0.77	0.76
55	assign (segid 3A4 and resid 39 and name CA) (segid 3A4 and resid 386 and name CA)	8.85	0.69	0.68
	assign (segid 3A4 and resid 39 and name CA) (segid 3A4 and resid 387 and name CA)	10.52	1.01	1.00
	assign (segid 3A4 and resid 39 and name CA) (segid 3A4 and resid 388 and name CA)	13.73	1.01	1.01
	assign (segid 3A4 and resid 39 and name CA) (segid 3A4 and resid 388 and name CB)	14.32	1.11	1.12
	assign (segid 3A4 and resid 39 and name CA) (segid 3A4 and resid 389 and name CA)	13.46	0.79	0.78
60	assign (segid 3A4 and resid 39 and name CA) (segid 3A4 and resid 389 and name CB)	12.91	0.74	0.74
	assign (segid 3A4 and resid 39 and name CA) (segid 3A4 and resid 390 and name CA)	13.02	0.77	0.77
	assign (segid 3A4 and resid 39 and name CA) (segid 3A4 and resid 390 and name CB)	13.09	0.80	0.80
	assign (segid 3A4 and resid 39 and name CA) (segid 3A4 and resid 391 and name CA)	15.68	0.78	0.78
	assign (segid 3A4 and resid 39 and name CA) (segid 3A4 and resid 391 and name CB)	15.72	0.76	0.76
65	assign (segid 3A4 and resid 39 and name CA) (segid 3A4 and resid 394 and name CA)	17.87	0.80	0.80
	assign (segid 3A4 and resid 39 and name CA) (segid 3A4 and resid 39 and name C)	1.51	0.01	0.01
	assign (segid 3A4 and resid 39 and name CA) (segid 3A4 and resid 39 and name CB)	1.55	0.02	0.02
	assign (segid 3A4 and resid 39 and name CA) (segid 3A4 and resid 39 and name O)	2.37	0.04	0.04
	assign (segid 3A4 and resid 39 and name CA) (segid 3A4 and resid 40 and name C)	1.38	0.03	0.03
70	assign (segid 3A4 and resid 39 and name CA) (segid 3A4 and resid 40 and name CA)	3.82	0.02	0.03
	assign (segid 3A4 and resid 39 and name CA) (segid 3A4 and resid 40 and name CB)	4.90	0.05	0.06
	assign (segid 3A4 and resid 39 and name CA) (segid 3A4 and resid 40 and name N)	2.46	0.04	0.03
	assign (segid 3A4 and resid 39 and name CA) (segid 3A4 and resid 40 and name O)	5.27	0.08	0.08
	assign (segid 3A4 and resid 39 and name CA) (segid 3A4 and resid 41 and name C)	5.42	0.13	0.12
75	assign (segid 3A4 and resid 39 and name CA) (segid 3A4 and resid 41 and name CA)	5.35	0.09	0.09
	assign (segid 3A4 and resid 39 and name CA) (segid 3A4 and resid 41 and name CB)	5.70	0.11	0.11
	assign (segid 3A4 and resid 39 and name CA) (segid 3A4 and resid 41 and name N)	4.30	0.07	0.08
	assign (segid 3A4 and resid 39 and name CA) (segid 3A4 and resid 41 and name O)	6.55	0.14	0.14
	assign (segid 3A4 and resid 39 and name CA) (segid 3A4 and resid 42 and name C)	5.65	0.13	0.13
80	assign (segid 3A4 and resid 39 and name CA) (segid 3A4 and resid 42 and name CA)	5.12	0.17	0.17
	assign (segid 3A4 and resid 39 and name CA) (segid 3A4 and resid 42 and name CB)	4.55	0.19	0.19
	assign (segid 3A4 and resid 39 and name CA) (segid 3A4 and resid 42 and name N)	4.52	0.16	0.16
	assign (segid 3A4 and resid 39 and name CA) (segid 3A4 and resid 42 and name O)	6.83	0.16	0.16

	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 258 and name CB)	18.47	0.72	0.72
	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 310 and name CA)	17.83	0.45	0.45
	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 310 and name CB)	17.92	0.44	0.43
	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 311 and name CA)	17.91	0.46	0.46
5	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 312 and name CA)	18.64	0.55	0.54
	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 313 and name CA)	15.60	0.51	0.52
	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 313 and name CB)	15.48	0.46	0.46
	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 314 and name CA)	13.42	0.51	0.52
	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 314 and name CB)	13.74	0.49	0.49
10	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 315 and name CA)	15.48	0.61	0.60
	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 315 and name CB)	16.95	0.59	0.58
	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 316 and name CA)	15.94	0.77	0.77
	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 316 and name CB)	13.04	0.69	0.69
	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 317 and name CA)	15.03	0.94	0.94
	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 318 and name CB)	16.11	0.89	0.90
15	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 319 and name CA)	12.90	0.98	0.97
	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 319 and name CB)	12.72	1.09	1.09
	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 322 and name CA)	10.98	0.89	0.88
	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 323 and name CA)	11.44	0.33	0.34
20	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 323 and name CB)	10.35	0.40	0.40
	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 324 and name CA)	14.22	0.35	0.35
	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 324 and name CB)	15.62	0.32	0.32
	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 325 and name CA)	14.77	0.39	0.40
	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 325 and name CB)	14.78	0.36	0.36
25	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 326 and name CA)	17.77	0.46	0.45
	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 326 and name CB)	17.84	0.50	0.50
	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 327 and name CA)	18.96	0.41	0.42
	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 327 and name CB)	19.32	0.48	0.48
	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 328 and name CA)	18.56	0.51	0.50
30	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 329 and name CA)	15.75	0.69	0.68
	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 329 and name CB)	14.62	0.68	0.68
	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 330 and name CA)	14.97	0.87	0.87
	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 330 and name CB)	16.14	0.93	0.92
	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 331 and name CA)	11.50	0.87	0.86
35	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 331 and name CB)	10.46	0.86	0.85
	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 332 and name CA)	12.03	0.99	0.99
	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 333 and name CA)	15.51	0.85	0.84
	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 335 and name CA)	15.04	0.76	0.75
	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 336 and name CA)	16.60	0.59	0.59
40	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 336 and name CB)	18.10	0.61	0.60
	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 337 and name CA)	15.40	0.49	0.48
	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 337 and name CB)	14.03	0.46	0.46
	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 338 and name CA)	18.46	0.37	0.37
	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 339 and name CA)	19.13	0.29	0.29
45	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 340 and name CA)	18.84	0.44	0.43
	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 341 and name CA)	16.38	0.37	0.37
	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 341 and name CB)	15.88	0.44	0.44
	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 342 and name CA)	14.19	0.30	0.30
50	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 343 and name CA)	10.49	0.25	0.25
	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 343 and name CB)	9.72	0.38	0.37
	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 344 and name C)	7.65	0.19	0.18
	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 344 and name CB)	9.06	0.15	0.14
	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 344 and name CB)	10.04	0.25	0.24
	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 344 and name C)	7.37	0.24	0.24
55	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 345 and name C)	5.79	0.58	0.59
	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 345 and name CA)	5.55	0.35	0.35
	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 345 and name CB)	5.01	0.32	0.32
	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 345 and name N)	6.89	0.25	0.24
	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 346 and name C)	5.91	0.71	0.72
60	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 346 and name CA)	6.51	0.64	0.64
	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 346 and name CB)	7.21	0.58	0.57
	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 346 and name N)	5.77	0.53	0.53
	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 346 and name O)	5.50	0.75	0.76
	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 347 and name CA)	6.28	0.73	0.74
65	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 347 and name CB)	7.15	0.76	0.76
	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 348 and name CA)	9.22	0.73	0.74
	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 349 and name CA)	8.05	0.62	0.62
	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 349 and name CB)	7.71	0.65	0.65
	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 350 and name CA)	5.90	0.45	0.44
70	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 350 and name CB)	4.87	0.58	0.57
	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 350 and name N)	6.31	0.47	0.47
	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 351 and name CA)	9.12	0.49	0.49
	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 352 and name CA)	11.15	0.45	0.45
	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 352 and name CB)	11.70	0.51	0.51
	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 353 and name CA)	10.08	0.44	0.44
75	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 353 and name CB)	8.89	0.53	0.53
	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 354 and name CA)	13.61	0.47	0.46
	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 354 and name CB)	14.58	0.44	0.44
	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 355 and name CA)	13.06	0.78	0.77
	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 355 and name CB)	12.38	0.87	0.87
80	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 356 and name CA)	11.95	0.72	0.72
	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 356 and name CB)	10.55	0.71	0.71
	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 357 and name CA)	14.10	0.68	0.68

	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 357 and name CB)	13.63	0.67	0.68
	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 358 and name CA)	17.57	0.66	0.66
	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 358 and name CB)	18.76	0.69	0.69
	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 359 and name CA)	18.88	0.63	0.62
	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 360 and name CA)	15.73	0.56	0.57
5	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 360 and name CB)	14.53	0.62	0.61
	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 361 and name CA)	17.89	0.55	0.54
	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 361 and name CB)	18.44	0.58	0.57
	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 381 and name CA)	9.85	0.49	0.48
	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 382 and name CA)	7.84	0.54	0.53
10	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 382 and name CB)	6.35	0.54	0.55
	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 383 and name CA)	10.55	0.54	0.54
	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 384 and name CA)	11.83	0.63	0.64
	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 384 and name CB)	12.92	0.60	0.60
	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 385 and name CA)	8.91	0.82	0.81
15	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 386 and name CA)	8.66	0.70	0.69
	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 387 and name CA)	10.81	0.98	0.99
	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 388 and name CA)	14.07	0.96	0.95
	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 388 and name CB)	14.79	1.07	1.06
	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 389 and name CA)	13.48	0.76	0.77
20	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 389 and name CB)	12.97	0.73	0.73
	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 390 and name CA)	12.72	0.78	0.78
	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 390 and name CB)	12.82	0.81	0.82
	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 391 and name CA)	15.10	0.78	0.78
	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 391 and name CB)	15.00	0.76	0.77
25	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 394 and name CA)	18.14	0.74	0.75
	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 394 and name CB)	17.09	0.82	0.83
	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 40 and name C)	5.44	0.07	0.07
	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 40 and name CA)	4.52	0.08	0.07
	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 40 and name CB)	5.43	0.13	0.12
30	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 40 and name N)	3.19	0.08	0.08
	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 40 and name O)	6.30	0.12	0.11
	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 41 and name C)	6.86	0.13	0.13
	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 41 and name CA)	6.75	0.07	0.06
	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 41 and name CB)	7.16	0.08	0.08
35	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 41 and name N)	5.58	0.04	0.04
	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 42 and name C)	6.84	0.18	0.18
	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 42 and name CA)	6.49	0.22	0.21
	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 42 and name CB)	5.82	0.28	0.27
	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 42 and name N)	5.99	0.18	0.17
40	assign (segid 3A4 and resid 39 and name CB) (segid 3A4 and resid 42 and name O)	6.86	0.49	0.48
	assign (segid 3A4 and resid 39 and name N) (segid 3A4 and resid 345 and name CA)	6.38	0.56	0.56
	assign (segid 3A4 and resid 39 and name N) (segid 3A4 and resid 350 and name CB)	6.62	0.62	0.62
	assign (segid 3A4 and resid 39 and name N) (segid 3A4 and resid 39 and name C)	2.43	0.06	0.06
	assign (segid 3A4 and resid 39 and name N) (segid 3A4 and resid 39 and name CA)	1.46	0.01	0.01
45	assign (segid 3A4 and resid 39 and name N) (segid 3A4 and resid 39 and name CB)	2.47	0.02	0.02
	assign (segid 3A4 and resid 39 and name N) (segid 3A4 and resid 39 and name O)	3.44	0.08	0.07
	assign (segid 3A4 and resid 39 and name N) (segid 3A4 and resid 40 and name C)	4.67	0.05	0.06
	assign (segid 3A4 and resid 39 and name N) (segid 3A4 and resid 40 and name CA)	4.23	0.06	0.06
	assign (segid 3A4 and resid 39 and name N) (segid 3A4 and resid 40 and name CB)	5.02	0.06	0.06
50	assign (segid 3A4 and resid 39 and name N) (segid 3A4 and resid 40 and name N)	2.84	0.06	0.07
	assign (segid 3A4 and resid 39 and name N) (segid 3A4 and resid 40 and name O)	5.74	0.07	0.06
	assign (segid 3A4 and resid 39 and name N) (segid 3A4 and resid 41 and name C)	5.54	0.08	0.07
	assign (segid 3A4 and resid 39 and name N) (segid 3A4 and resid 41 and name CA)	5.20	0.06	0.06
	assign (segid 3A4 and resid 39 and name N) (segid 3A4 and resid 41 and name CB)	5.19	0.07	0.07
55	assign (segid 3A4 and resid 39 and name N) (segid 3A4 and resid 41 and name N)	4.24	0.08	0.07
	assign (segid 3A4 and resid 39 and name N) (segid 3A4 and resid 41 and name O)	6.75	0.08	0.09
	assign (segid 3A4 and resid 39 and name N) (segid 3A4 and resid 42 and name C)	6.40	0.07	0.07
	assign (segid 3A4 and resid 39 and name N) (segid 3A4 and resid 42 and name CA)	5.59	0.10	0.10
	assign (segid 3A4 and resid 39 and name N) (segid 3A4 and resid 42 and name CB)	5.07	0.11	0.10
60	assign (segid 3A4 and resid 39 and name N) (segid 3A4 and resid 42 and name N)	4.76	0.10	0.10
	assign (segid 3A4 and resid 39 and name N) (segid 3A4 and resid 42 and name O)	7.58	0.08	0.09
	assign (segid 3A4 and resid 39 and name O) (segid 3A4 and resid 345 and name CB)	5.68	0.75	0.74
	assign (segid 3A4 and resid 39 and name O) (segid 3A4 and resid 39 and name CB)	3.35	0.03	0.02
	assign (segid 3A4 and resid 39 and name O) (segid 3A4 and resid 40 and name C)	2.89	0.08	0.08
65	assign (segid 3A4 and resid 39 and name O) (segid 3A4 and resid 40 and name CA)	2.74	0.04	0.04
	assign (segid 3A4 and resid 39 and name O) (segid 3A4 and resid 40 and name CB)	4.23	0.04	0.03
	assign (segid 3A4 and resid 39 and name O) (segid 3A4 and resid 40 and name N)	2.22	0.01	0.02
	assign (segid 3A4 and resid 39 and name O) (segid 3A4 and resid 40 and name O)	3.36	0.12	0.11
	assign (segid 3A4 and resid 39 and name O) (segid 3A4 and resid 41 and name C)	4.00	0.16	0.17
70	assign (segid 3A4 and resid 39 and name O) (segid 3A4 and resid 41 and name CA)	4.25	0.17	0.16
	assign (segid 3A4 and resid 39 and name O) (segid 3A4 and resid 41 and name CB)	5.17	0.18	0.17
	assign (segid 3A4 and resid 39 and name O) (segid 3A4 and resid 41 and name N)	3.30	0.15	0.16
	assign (segid 3A4 and resid 39 and name O) (segid 3A4 and resid 41 and name O)	4.93	0.18	0.17
	assign (segid 3A4 and resid 39 and name O) (segid 3A4 and resid 42 and name C)	3.80	0.10	0.10
75	assign (segid 3A4 and resid 39 and name O) (segid 3A4 and resid 42 and name CA)	3.78	0.14	0.14
	assign (segid 3A4 and resid 39 and name O) (segid 3A4 and resid 42 and name CB)	3.77	0.13	0.13
	assign (segid 3A4 and resid 39 and name O) (segid 3A4 and resid 42 and name N)	3.27	0.17	0.17
	assign (segid 3A4 and resid 39 and name O) (segid 3A4 and resid 42 and name O)	4.95	0.10	0.11
80	assign (segid 3A4 and resid 400 and name C) (segid 3A4 and resid 400 and name CB)	2.49	0.01	0.02
	assign (segid 3A4 and resid 400 and name C) (segid 3A4 and resid 400 and name O)	1.23	0.01	0.01
	assign (segid 3A4 and resid 400 and name C) (segid 3A4 and resid 401 and name C)	3.04	0.05	0.04
	assign (segid 3A4 and resid 400 and name C) (segid 3A4 and resid 401 and name CA)	2.42	0.01	0.01

	assign (segid 3A4 and resid 400 and name C) (segid 3A4 and resid 401 and name N)	1.32	0.02	0.02
	assign (segid 3A4 and resid 400 and name C) (segid 3A4 and resid 401 and name O)	3.83	0.09	0.08
	assign (segid 3A4 and resid 400 and name C) (segid 3A4 and resid 402 and name C)	4.65	0.06	0.05
	assign (segid 3A4 and resid 400 and name C) (segid 3A4 and resid 402 and name CA)	4.57	0.08	0.07
	assign (segid 3A4 and resid 400 and name C) (segid 3A4 and resid 402 and name CB)	5.36	0.09	0.09
5	assign (segid 3A4 and resid 400 and name C) (segid 3A4 and resid 402 and name N)	3.38	0.06	0.06
	assign (segid 3A4 and resid 400 and name C) (segid 3A4 and resid 402 and name O)	5.70	0.08	0.08
	assign (segid 3A4 and resid 400 and name C) (segid 3A4 and resid 403 and name C)	4.93	0.08	0.08
	assign (segid 3A4 and resid 400 and name C) (segid 3A4 and resid 403 and name CA)	4.69	0.10	0.11
	assign (segid 3A4 and resid 400 and name C) (segid 3A4 and resid 403 and name CB)	4.56	0.19	0.18
10	assign (segid 3A4 and resid 400 and name C) (segid 3A4 and resid 403 and name N)	3.97	0.10	0.10
	assign (segid 3A4 and resid 400 and name C) (segid 3A4 and resid 403 and name O)	6.13	0.10	0.10
	assign (segid 3A4 and resid 400 and name C) (segid 3A4 and resid 404 and name C)	5.98	0.20	0.20
	assign (segid 3A4 and resid 400 and name C) (segid 3A4 and resid 404 and name CA)	4.94	0.13	0.13
	assign (segid 3A4 and resid 400 and name C) (segid 3A4 and resid 404 and name CB)	4.46	0.17	0.16
15	assign (segid 3A4 and resid 400 and name C) (segid 3A4 and resid 404 and name N)	4.12	0.10	0.11
	assign (segid 3A4 and resid 400 and name C) (segid 3A4 and resid 404 and name O)	7.14	0.18	0.19
	assign (segid 3A4 and resid 400 and name C) (segid 3A4 and resid 405 and name CA)	7.07	0.29	0.29
	assign (segid 3A4 and resid 400 and name C) (segid 3A4 and resid 405 and name CB)	7.10	0.34	0.35
	assign (segid 3A4 and resid 400 and name C) (segid 3A4 and resid 405 and name N)	5.80	0.25	0.26
20	assign (segid 3A4 and resid 400 and name C) (segid 3A4 and resid 400 and name C)	1.52	0.00	0.01
	assign (segid 3A4 and resid 400 and name CA) (segid 3A4 and resid 400 and name CB)	1.52	0.01	0.01
	assign (segid 3A4 and resid 400 and name CA) (segid 3A4 and resid 400 and name O)	2.38	0.03	0.02
	assign (segid 3A4 and resid 400 and name CA) (segid 3A4 and resid 401 and name C)	4.43	0.03	0.04
	assign (segid 3A4 and resid 400 and name CA) (segid 3A4 and resid 401 and name CA)	3.81	0.03	0.03
25	assign (segid 3A4 and resid 400 and name CA) (segid 3A4 and resid 401 and name N)	2.45	0.05	0.05
	assign (segid 3A4 and resid 400 and name CA) (segid 3A4 and resid 401 and name O)	5.29	0.09	0.08
	assign (segid 3A4 and resid 400 and name CA) (segid 3A4 and resid 402 and name C)	5.58	0.05	0.06
	assign (segid 3A4 and resid 400 and name CA) (segid 3A4 and resid 402 and name CA)	5.57	0.06	0.07
	assign (segid 3A4 and resid 400 and name CA) (segid 3A4 and resid 402 and name CB)	6.06	0.11	0.11
30	assign (segid 3A4 and resid 400 and name CA) (segid 3A4 and resid 402 and name N)	4.49	0.05	0.05
	assign (segid 3A4 and resid 400 and name CA) (segid 3A4 and resid 402 and name O)	6.69	0.07	0.08
	assign (segid 3A4 and resid 400 and name CA) (segid 3A4 and resid 403 and name C)	5.69	0.11	0.12
	assign (segid 3A4 and resid 400 and name CA) (segid 3A4 and resid 403 and name CA)	5.23	0.08	0.07
	assign (segid 3A4 and resid 400 and name CA) (segid 3A4 and resid 403 and name CB)	4.65	0.13	0.13
35	assign (segid 3A4 and resid 400 and name CA) (segid 3A4 and resid 403 and name N)	4.68	0.07	0.07
	assign (segid 3A4 and resid 400 and name CA) (segid 3A4 and resid 403 and name O)	6.88	0.12	0.12
	assign (segid 3A4 and resid 400 and name CA) (segid 3A4 and resid 404 and name C)	7.15	0.24	0.25
	assign (segid 3A4 and resid 400 and name CA) (segid 3A4 and resid 404 and name CA)	5.96	0.22	0.22
	assign (segid 3A4 and resid 400 and name CA) (segid 3A4 and resid 404 and name CB)	5.55	0.28	0.27
40	assign (segid 3A4 and resid 400 and name CA) (segid 3A4 and resid 404 and name N)	5.05	0.18	0.19
	assign (segid 3A4 and resid 400 and name CA) (segid 3A4 and resid 405 and name CA)	8.44	0.28	0.28
	assign (segid 3A4 and resid 400 and name CA) (segid 3A4 and resid 405 and name CB)	8.55	0.33	0.32
	assign (segid 3A4 and resid 400 and name CA) (segid 3A4 and resid 405 and name N)	7.12	0.27	0.28
	assign (segid 3A4 and resid 400 and name CA) (segid 3A4 and resid 406 and name CA)	9.89	0.21	0.22
45	assign (segid 3A4 and resid 400 and name CA) (segid 3A4 and resid 407 and name CA)	10.61	0.17	0.17
	assign (segid 3A4 and resid 400 and name CA) (segid 3A4 and resid 407 and name CB)	9.92	0.14	0.13
	assign (segid 3A4 and resid 400 and name CA) (segid 3A4 and resid 408 and name CA)	11.91	0.16	0.17
	assign (segid 3A4 and resid 400 and name CA) (segid 3A4 and resid 408 and name CB)	11.45	0.16	0.16
	assign (segid 3A4 and resid 400 and name CA) (segid 3A4 and resid 409 and name CA)	14.26	0.35	0.34
50	assign (segid 3A4 and resid 400 and name CA) (segid 3A4 and resid 409 and name CB)	14.13	0.50	0.49
	assign (segid 3A4 and resid 400 and name CA) (segid 3A4 and resid 410 and name CA)	15.55	0.47	0.47
	assign (segid 3A4 and resid 400 and name CA) (segid 3A4 and resid 411 and name CA)	16.56	0.34	0.34
	assign (segid 3A4 and resid 400 and name CA) (segid 3A4 and resid 411 and name CB)	15.79	0.40	0.40
	assign (segid 3A4 and resid 400 and name CA) (segid 3A4 and resid 412 and name CA)	17.90	0.43	0.44
55	assign (segid 3A4 and resid 400 and name CA) (segid 3A4 and resid 433 and name CA)	18.82	0.52	0.52
	assign (segid 3A4 and resid 400 and name CA) (segid 3A4 and resid 434 and name CA)	17.50	0.66	0.66
	assign (segid 3A4 and resid 400 and name CA) (segid 3A4 and resid 435 and name CA)	18.29	0.52	0.52
	assign (segid 3A4 and resid 400 and name CB) (segid 3A4 and resid 401 and name C)	5.43	0.07	0.07
	assign (segid 3A4 and resid 400 and name CB) (segid 3A4 and resid 401 and name CA)	4.46	0.08	0.07
60	assign (segid 3A4 and resid 400 and name CB) (segid 3A4 and resid 401 and name N)	3.14	0.09	0.10
	assign (segid 3A4 and resid 400 and name CB) (segid 3A4 and resid 401 and name O)	6.25	0.09	0.10
	assign (segid 3A4 and resid 400 and name CB) (segid 3A4 and resid 402 and name C)	6.99	0.05	0.05
	assign (segid 3A4 and resid 400 and name CB) (segid 3A4 and resid 402 and name CA)	6.91	0.08	0.07
	assign (segid 3A4 and resid 400 and name CB) (segid 3A4 and resid 402 and name CB)	7.44	0.10	0.10
65	assign (segid 3A4 and resid 400 and name CB) (segid 3A4 and resid 402 and name N)	5.70	0.07	0.06
	assign (segid 3A4 and resid 400 and name CB) (segid 3A4 and resid 403 and name C)	6.91	0.11	0.12
	assign (segid 3A4 and resid 400 and name CB) (segid 3A4 and resid 403 and name CA)	6.62	0.09	0.09
	assign (segid 3A4 and resid 400 and name CB) (segid 3A4 and resid 403 and name CB)	5.98	0.16	0.17
	assign (segid 3A4 and resid 400 and name CB) (segid 3A4 and resid 403 and name N)	6.13	0.08	0.09
70	assign (segid 3A4 and resid 400 and name CB) (segid 3A4 and resid 403 and name CA)	6.79	0.22	0.22
	assign (segid 3A4 and resid 400 and name CB) (segid 3A4 and resid 404 and name CB)	6.09	0.29	0.29
	assign (segid 3A4 and resid 400 and name CB) (segid 3A4 and resid 404 and name N)	6.12	0.17	0.17
	assign (segid 3A4 and resid 400 and name CB) (segid 3A4 and resid 405 and name CA)	9.38	0.34	0.34
	assign (segid 3A4 and resid 400 and name CB) (segid 3A4 and resid 405 and name CB)	9.48	0.39	0.38
75	assign (segid 3A4 and resid 400 and name CB) (segid 3A4 and resid 406 and name CA)	11.16	0.23	0.23
	assign (segid 3A4 and resid 400 and name CB) (segid 3A4 and resid 407 and name CA)	11.67	0.16	0.17
	assign (segid 3A4 and resid 400 and name CB) (segid 3A4 and resid 407 and name CB)	10.91	0.15	0.15
	assign (segid 3A4 and resid 400 and name CB) (segid 3A4 and resid 408 and name CA)	12.68	0.20	0.20
	assign (segid 3A4 and resid 400 and name CB) (segid 3A4 and resid 408 and name CB)	12.10	0.21	0.22
80	assign (segid 3A4 and resid 400 and name CB) (segid 3A4 and resid 409 and name CA)	15.20	0.33	0.33
	assign (segid 3A4 and resid 400 and name CB) (segid 3A4 and resid 409 and name CB)	15.12	0.47	0.46
	assign (segid 3A4 and resid 400 and name CB) (segid 3A4 and resid 410 and name CA)	16.64	0.43	0.44

	assign (segid 3A4 and resid 400 and name CB)	(segid 3A4 and resid 411 and name CA)	17.44	0.33	0.33
	assign (segid 3A4 and resid 400 and name CB)	(segid 3A4 and resid 411 and name CB)	16.59	0.40	0.41
	assign (segid 3A4 and resid 400 and name CB)	(segid 3A4 and resid 412 and name CA)	18.64	0.46	0.46
	assign (segid 3A4 and resid 400 and name CB)	(segid 3A4 and resid 433 and name CA)	17.93	0.58	0.59
5	assign (segid 3A4 and resid 100 and name CB)	(segid 3A4 and resid 434 and name CA)	16.67	0.72	0.72
	assign (segid 3A4 and resid 400 and name CB)	(segid 3A4 and resid 435 and name CA)	17.60	0.60	0.59
	assign (segid 3A4 and resid 400 and name CB)	(segid HEM and resid 1 and name CMC)	7.19	0.27	0.28
	assign (segid 3A4 and resid 400 and name N)	(segid 3A4 and resid 400 and name C)	2.46	0.02	0.01
	assign (segid 3A4 and resid 400 and name N)	(segid 3A4 and resid 400 and name CA)	1.45	0.01	0.01
10	assign (segid 3A4 and resid 400 and name N)	(segid 3A4 and resid 400 and name CB)	2.43	0.05	0.05
	assign (segid 3A4 and resid 400 and name N)	(segid 3A4 and resid 400 and name O)	3.47	0.04	0.04
	assign (segid 3A4 and resid 400 and name N)	(segid 3A4 and resid 401 and name C)	4.75	0.04	0.03
	assign (segid 3A4 and resid 400 and name N)	(segid 3A4 and resid 401 and name CA)	4.25	0.04	0.04
	assign (segid 3A4 and resid 400 and name N)	(segid 3A4 and resid 401 and name N)	2.86	0.04	0.04
15	assign (segid 3A4 and resid 400 and name N)	(segid 3A4 and resid 401 and name O)	5.79	0.06	0.05
	assign (segid 3A4 and resid 400 and name N)	(segid 3A4 and resid 402 and name C)	5.68	0.05	0.05
	assign (segid 3A4 and resid 400 and name N)	(segid 3A4 and resid 402 and name CA)	5.45	0.06	0.05
	assign (segid 3A4 and resid 400 and name N)	(segid 3A4 and resid 402 and name CB)	5.57	0.11	0.10
	assign (segid 3A4 and resid 400 and name N)	(segid 3A4 and resid 402 and name N)	4.43	0.04	0.05
20	assign (segid 3A4 and resid 400 and name N)	(segid 3A4 and resid 402 and name O)	6.87	0.06	0.06
	assign (segid 3A4 and resid 400 and name N)	(segid 3A4 and resid 403 and name C)	6.36	0.14	0.13
	assign (segid 3A4 and resid 400 and name N)	(segid 3A4 and resid 403 and name CA)	5.58	0.08	0.08
	assign (segid 3A4 and resid 400 and name N)	(segid 3A4 and resid 403 and name CB)	5.00	0.08	0.09
	assign (segid 3A4 and resid 400 and name N)	(segid 3A4 and resid 403 and name N)	4.84	0.07	0.07
25	assign (segid 3A4 and resid 400 and name N)	(segid 3A4 and resid 403 and name O)	7.57	0.13	0.12
	assign (segid 3A4 and resid 400 and name N)	(segid 3A4 and resid 404 and name CA)	7.01	0.21	0.20
	assign (segid 3A4 and resid 400 and name N)	(segid 3A4 and resid 404 and name CB)	6.74	0.23	0.23
	assign (segid 3A4 and resid 400 and name N)	(segid 3A4 and resid 404 and name N)	5.93	0.19	0.18
	assign (segid 3A4 and resid 400 and name O)	(segid 3A4 and resid 400 and name CB)	3.29	0.10	0.09
30	assign (segid 3A4 and resid 400 and name O)	(segid 3A4 and resid 401 and name C)	2.99	0.07	0.08
	assign (segid 3A4 and resid 400 and name O)	(segid 3A4 and resid 401 and name CA)	2.74	0.03	0.03
	assign (segid 3A4 and resid 400 and name O)	(segid 3A4 and resid 401 and name N)	2.23	0.01	0.01
	assign (segid 3A4 and resid 400 and name O)	(segid 3A4 and resid 401 and name O)	3.41	0.12	0.12
	assign (segid 3A4 and resid 400 and name O)	(segid 3A4 and resid 402 and name C)	4.25	0.14	0.14
35	assign (segid 3A4 and resid 400 and name O)	(segid 3A4 and resid 402 and name CA)	4.51	0.15	0.14
	assign (segid 3A4 and resid 400 and name O)	(segid 3A4 and resid 402 and name CB)	5.53	0.14	0.14
	assign (segid 3A4 and resid 400 and name O)	(segid 3A4 and resid 402 and name N)	3.54	0.11	0.12
	assign (segid 3A4 and resid 400 and name O)	(segid 3A4 and resid 402 and name O)	5.14	0.16	0.16
	assign (segid 3A4 and resid 400 and name O)	(segid 3A4 and resid 403 and name C)	3.96	0.12	0.11
40	assign (segid 3A4 and resid 400 and name O)	(segid 3A4 and resid 403 and name CA)	4.01	0.19	0.19
	assign (segid 3A4 and resid 400 and name O)	(segid 3A4 and resid 403 and name CB)	4.00	0.29	0.29
	assign (segid 3A4 and resid 400 and name O)	(segid 3A4 and resid 403 and name N)	3.55	0.20	0.19
	assign (segid 3A4 and resid 400 and name O)	(segid 3A4 and resid 403 and name O)	5.10	0.11	0.11
	assign (segid 3A4 and resid 400 and name O)	(segid 3A4 and resid 404 and name C)	4.86	0.24	0.24
45	assign (segid 3A4 and resid 400 and name O)	(segid 3A4 and resid 404 and name CA)	3.75	0.15	0.15
	assign (segid 3A4 and resid 400 and name O)	(segid 3A4 and resid 404 and name CB)	3.33	0.19	0.19
	assign (segid 3A4 and resid 400 and name O)	(segid 3A4 and resid 404 and name N)	3.02	0.12	0.12
	assign (segid 3A4 and resid 400 and name O)	(segid 3A4 and resid 404 and name O)	6.00	0.22	0.21
50	assign (segid 3A4 and resid 400 and name O)	(segid 3A4 and resid 405 and name C)	7.08	0.32	0.32
	assign (segid 3A4 and resid 400 and name O)	(segid 3A4 and resid 405 and name CA)	6.18	0.35	0.35
	assign (segid 3A4 and resid 400 and name O)	(segid 3A4 and resid 405 and name CB)	6.42	0.40	0.40
	assign (segid 3A4 and resid 400 and name O)	(segid 3A4 and resid 405 and name N)	4.83	0.32	0.33
	assign (segid 3A4 and resid 400 and name O)	(segid 3A4 and resid 406 and name N)	6.83	0.30	0.29
	assign (segid 3A4 and resid 401 and name C)	(segid 3A4 and resid 401 and name O)	1.24	0.02	0.01
55	assign (segid 3A4 and resid 401 and name C)	(segid 3A4 and resid 402 and name C)	3.05	0.03	0.04
	assign (segid 3A4 and resid 401 and name C)	(segid 3A4 and resid 402 and name CA)	2.43	0.01	0.01
	assign (segid 3A4 and resid 401 and name C)	(segid 3A4 and resid 402 and name CB)	3.70	0.03	0.02
	assign (segid 3A4 and resid 401 and name C)	(segid 3A4 and resid 402 and name N)	1.32	0.03	0.02
	assign (segid 3A4 and resid 401 and name C)	(segid 3A4 and resid 402 and name O)	3.89	0.06	0.06
60	assign (segid 3A4 and resid 401 and name C)	(segid 3A4 and resid 403 and name C)	4.63	0.08	0.07
	assign (segid 3A4 and resid 401 and name C)	(segid 3A4 and resid 403 and name CA)	4.55	0.09	0.08
	assign (segid 3A4 and resid 401 and name C)	(segid 3A4 and resid 403 and name CB)	5.33	0.11	0.12
	assign (segid 3A4 and resid 401 and name C)	(segid 3A4 and resid 403 and name N)	3.36	0.09	0.09
	assign (segid 3A4 and resid 401 and name C)	(segid 3A4 and resid 403 and name O)	5.66	0.07	0.07
65	assign (segid 3A4 and resid 401 and name C)	(segid 3A4 and resid 404 and name C)	4.95	0.06	0.05
	assign (segid 3A4 and resid 401 and name C)	(segid 3A4 and resid 404 and name CA)	4.68	0.12	0.13
	assign (segid 3A4 and resid 401 and name C)	(segid 3A4 and resid 404 and name CB)	4.50	0.18	0.19
	assign (segid 3A4 and resid 401 and name C)	(segid 3A4 and resid 404 and name N)	3.96	0.13	0.13
	assign (segid 3A4 and resid 401 and name C)	(segid 3A4 and resid 404 and name O)	6.15	0.04	0.04
70	assign (segid 3A4 and resid 401 and name C)	(segid 3A4 and resid 405 and name C)	5.94	0.13	0.14
	assign (segid 3A4 and resid 401 and name C)	(segid 3A4 and resid 405 and name CA)	5.00	0.11	0.11
	assign (segid 3A4 and resid 401 and name C)	(segid 3A4 and resid 405 and name CB)	4.57	0.19	0.18
	assign (segid 3A4 and resid 401 and name C)	(segid 3A4 and resid 405 and name N)	4.15	0.05	0.06
	assign (segid 3A4 and resid 401 and name C)	(segid 3A4 and resid 405 and name O)	7.11	0.15	0.14
75	assign (segid 3A4 and resid 401 and name C)	(segid 3A4 and resid 406 and name CA)	6.98	0.24	0.24
	assign (segid 3A4 and resid 401 and name C)	(segid 3A4 and resid 406 and name N)	5.74	0.20	0.21
	assign (segid 3A4 and resid 401 and name C)	(segid 3A4 and resid 407 and name N)	7.73	0.14	0.13
	assign (segid 3A4 and resid 401 and name CA)	(segid 3A4 and resid 401 and name C)	1.52	0.02	0.02
80	assign (segid 3A4 and resid 401 and name CA)	(segid 3A4 and resid 401 and name O)	2.38	0.02	0.02
	assign (segid 3A4 and resid 401 and name CA)	(segid 3A4 and resid 402 and name C)	4.45	0.03	0.02
	assign (segid 3A4 and resid 401 and name CA)	(segid 3A4 and resid 402 and name CA)	3.81	0.02	0.02
	assign (segid 3A4 and resid 401 and name CA)	(segid 3A4 and resid 402 and name CB)	4.86	0.03	0.02
	assign (segid 3A4 and resid 401 and name CA)	(segid 3A4 and resid 402 and name N)	2.43	0.01	0.02

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	assign (segid 3A4 and resid 402 and name C) (segid 3A4 and resid 403 and name C)	3.03	0.04	0.03
	assign (segid 3A4 and resid 402 and name C) (segid 3A4 and resid 403 and name CA)	2.42	0.01	0.02
	assign (segid 3A4 and resid 402 and name C) (segid 3A4 and resid 403 and name CB)	3.70	0.02	0.03
	assign (segid 3A4 and resid 402 and name C) (segid 3A4 and resid 403 and name N)	1.32	0.01	0.01
5	assign (segid 3A4 and resid 402 and name C) (segid 3A4 and resid 403 and name O)	3.83	0.07	0.07
	assign (segid 3A4 and resid 402 and name C) (segid 3A4 and resid 404 and name C)	4.62	0.07	0.07
	assign (segid 3A4 and resid 402 and name C) (segid 3A4 and resid 404 and name CA)	4.54	0.09	0.10
	assign (segid 3A4 and resid 402 and name C) (segid 3A4 and resid 404 and name CB)	5.31	0.11	0.12
	assign (segid 3A4 and resid 402 and name C) (segid 3A4 and resid 404 and name N)	3.36	0.11	0.11
	assign (segid 3A4 and resid 402 and name C) (segid 3A4 and resid 404 and name O)	5.61	0.05	0.04
10	assign (segid 3A4 and resid 402 and name C) (segid 3A4 and resid 405 and name C)	4.94	0.09	0.08
	assign (segid 3A4 and resid 402 and name C) (segid 3A4 and resid 405 and name CA)	4.79	0.12	0.11
	assign (segid 3A4 and resid 402 and name C) (segid 3A4 and resid 405 and name CB)	4.78	0.15	0.16
	assign (segid 3A4 and resid 402 and name C) (segid 3A4 and resid 405 and name N)	4.05	0.14	0.14
	assign (segid 3A4 and resid 402 and name C) (segid 3A4 and resid 405 and name O)	6.11	0.10	0.11
15	assign (segid 3A4 and resid 402 and name C) (segid 3A4 and resid 406 and name C)	5.92	0.10	0.10
	assign (segid 3A4 and resid 402 and name C) (segid 3A4 and resid 406 and name CA)	4.89	0.11	0.12
	assign (segid 3A4 and resid 402 and name C) (segid 3A4 and resid 406 and name N)	4.11	0.07	0.07
	assign (segid 3A4 and resid 402 and name C) (segid 3A4 and resid 406 and name O)	7.06	0.13	0.13
	assign (segid 3A4 and resid 402 and name C) (segid 3A4 and resid 407 and name CA)	7.08	0.11	0.12
20	assign (segid 3A4 and resid 402 and name C) (segid 3A4 and resid 407 and name CB)	7.10	0.14	0.14
	assign (segid 3A4 and resid 402 and name C) (segid 3A4 and resid 407 and name N)	5.83	0.12	0.12
	assign (segid 3A4 and resid 402 and name C) (segid 3A4 and resid 408 and name N)	7.77	0.05	0.06
	assign (segid 3A4 and resid 402 and name CA) (segid 3A4 and resid 402 and name C)	1.52	0.00	0.01
	assign (segid 3A4 and resid 402 and name CA) (segid 3A4 and resid 402 and name CB)	1.54	0.02	0.01
25	assign (segid 3A4 and resid 402 and name CA) (segid 3A4 and resid 402 and name O)	2.39	0.02	0.02
	assign (segid 3A4 and resid 402 and name CA) (segid 3A4 and resid 403 and name C)	4.42	0.03	0.03
	assign (segid 3A4 and resid 402 and name CA) (segid 3A4 and resid 403 and name CA)	3.81	0.01	0.01
	assign (segid 3A4 and resid 402 and name CA) (segid 3A4 and resid 403 and name CB)	4.86	0.04	0.04
	assign (segid 3A4 and resid 402 and name CA) (segid 3A4 and resid 403 and name N)	2.43	0.01	0.01
30	assign (segid 3A4 and resid 402 and name CA) (segid 3A4 and resid 403 and name O)	5.29	0.06	0.07
	assign (segid 3A4 and resid 402 and name CA) (segid 3A4 and resid 404 and name C)	5.58	0.09	0.08
	assign (segid 3A4 and resid 402 and name CA) (segid 3A4 and resid 404 and name CA)	5.54	0.11	0.11
	assign (segid 3A4 and resid 402 and name CA) (segid 3A4 and resid 404 and name CB)	5.99	0.15	0.15
	assign (segid 3A4 and resid 402 and name CA) (segid 3A4 and resid 404 and name N)	4.46	0.11	0.11
35	assign (segid 3A4 and resid 402 and name CA) (segid 3A4 and resid 404 and name O)	6.64	0.06	0.05
	assign (segid 3A4 and resid 402 and name CA) (segid 3A4 and resid 405 and name C)	5.69	0.10	0.11
	assign (segid 3A4 and resid 402 and name CA) (segid 3A4 and resid 405 and name CA)	5.33	0.13	0.12
	assign (segid 3A4 and resid 402 and name CA) (segid 3A4 and resid 405 and name CB)	4.89	0.17	0.17
	assign (segid 3A4 and resid 402 and name CA) (segid 3A4 and resid 405 and name N)	4.75	0.15	0.14
40	assign (segid 3A4 and resid 402 and name CA) (segid 3A4 and resid 405 and name O)	6.85	0.17	0.17
	assign (segid 3A4 and resid 402 and name CA) (segid 3A4 and resid 406 and name C)	7.11	0.12	0.13
	assign (segid 3A4 and resid 402 and name CA) (segid 3A4 and resid 406 and name CA)	5.92	0.15	0.15
	assign (segid 3A4 and resid 402 and name CA) (segid 3A4 and resid 406 and name N)	5.05	0.10	0.09
	assign (segid 3A4 and resid 402 and name CA) (segid 3A4 and resid 407 and name CA)	8.45	0.11	0.11
45	assign (segid 3A4 and resid 402 and name CA) (segid 3A4 and resid 407 and name CB)	8.54	0.11	0.12
	assign (segid 3A4 and resid 402 and name CA) (segid 3A4 and resid 407 and name N)	7.14	0.13	0.12
	assign (segid 3A4 and resid 402 and name CA) (segid 3A4 and resid 408 and name CA)	9.98	0.08	0.08
	assign (segid 3A4 and resid 402 and name CA) (segid 3A4 and resid 408 and name CB)	9.69	0.17	0.16
	assign (segid 3A4 and resid 402 and name CA) (segid 3A4 and resid 409 and name CA)	10.92	0.46	0.46
50	assign (segid 3A4 and resid 402 and name CA) (segid 3A4 and resid 409 and name CB)	10.35	0.65	0.65
	assign (segid 3A4 and resid 402 and name CA) (segid 3A4 and resid 410 and name CA)	12.24	0.47	0.48
	assign (segid 3A4 and resid 402 and name CA) (segid 3A4 and resid 411 and name CA)	14.34	0.24	0.24
	assign (segid 3A4 and resid 402 and name CA) (segid 3A4 and resid 411 and name CB)	14.05	0.28	0.27
	assign (segid 3A4 and resid 402 and name CA) (segid 3A4 and resid 412 and name CA)	15.54	0.25	0.25
55	assign (segid 3A4 and resid 402 and name CA) (segid 3A4 and resid 413 and name CA)	18.24	0.76	0.75
	assign (segid 3A4 and resid 402 and name CA) (segid 3A4 and resid 414 and name CA)	17.79	0.83	0.82
	assign (segid 3A4 and resid 402 and name CA) (segid 3A4 and resid 435 and name CA)	19.11	0.36	0.36
	assign (segid 3A4 and resid 402 and name CB) (segid 3A4 and resid 403 and name C)	5.44	0.04	0.04
60	assign (segid 3A4 and resid 402 and name CB) (segid 3A4 and resid 403 and name CA)	4.47	0.05	0.05
	assign (segid 3A4 and resid 402 and name CB) (segid 3A4 and resid 403 and name CB)	5.31	0.06	0.05
	assign (segid 3A4 and resid 402 and name CB) (segid 3A4 and resid 403 and name N)	3.15	0.06	0.05
	assign (segid 3A4 and resid 402 and name CB) (segid 3A4 and resid 403 and name O)	6.28	0.06	0.07
	assign (segid 3A4 and resid 402 and name CB) (segid 3A4 and resid 404 and name C)	7.00	0.07	0.08
	assign (segid 3A4 and resid 402 and name CB) (segid 3A4 and resid 404 and name CA)	6.90	0.10	0.10
65	assign (segid 3A4 and resid 402 and name CB) (segid 3A4 and resid 404 and name CB)	7.39	0.13	0.14
	assign (segid 3A4 and resid 402 and name CB) (segid 3A4 and resid 404 and name N)	5.69	0.10	0.10
	assign (segid 3A4 and resid 402 and name CB) (segid 3A4 and resid 405 and name C)	6.93	0.14	0.14
	assign (segid 3A4 and resid 402 and name CB) (segid 3A4 and resid 405 and name CA)	6.74	0.15	0.15
	assign (segid 3A4 and resid 402 and name CB) (segid 3A4 and resid 405 and name CB)	6.25	0.20	0.20
70	assign (segid 3A4 and resid 402 and name CB) (segid 3A4 and resid 405 and name N)	6.22	0.15	0.15
	assign (segid 3A4 and resid 402 and name CB) (segid 3A4 and resid 406 and name CA)	6.77	0.10	0.10
	assign (segid 3A4 and resid 402 and name CB) (segid 3A4 and resid 406 and name N)	6.14	0.07	0.07
	assign (segid 3A4 and resid 402 and name CB) (segid 3A4 and resid 407 and name CA)	9.45	0.13	0.12
	assign (segid 3A4 and resid 402 and name CB) (segid 3A4 and resid 407 and name CB)	9.53	0.16	0.16
75	assign (segid 3A4 and resid 402 and name CB) (segid 3A4 and resid 408 and name CA)	11.29	0.08	0.08
	assign (segid 3A4 and resid 402 and name CB) (segid 3A4 and resid 408 and name CB)	11.10	0.17	0.17
	assign (segid 3A4 and resid 402 and name CB) (segid 3A4 and resid 409 and name CA)	12.05	0.49	0.49
	assign (segid 3A4 and resid 402 and name CB) (segid 3A4 and resid 409 and name CB)	11.42	0.69	0.70
80	assign (segid 3A4 and resid 402 and name CB) (segid 3A4 and resid 410 and name CA)	13.11	0.50	0.51
	assign (segid 3A4 and resid 402 and name CB) (segid 3A4 and resid 411 and name CA)	15.40	0.28	0.29
	assign (segid 3A4 and resid 402 and name CB) (segid 3A4 and resid 411 and name CB)	15.15	0.30	0.30
	assign (segid 3A4 and resid 402 and name CB) (segid 3A4 and resid 412 and name CA)	16.76	0.26	0.26

5	assign (segid 3A4 and resid 402 and name N) (segid 3A4 and resid 402 and name C)	2.47	0.01	0.02
	assign (segid 3A4 and resid 402 and name N) (segid 3A4 and resid 402 and name CA)	1.46	0.01	0.01
	assign (segid 3A4 and resid 402 and name N) (segid 3A4 and resid 402 and name CB)	2.45	0.02	0.02
	assign (segid 3A4 and resid 402 and name N) (segid 3A4 and resid 402 and name O)	3.51	0.03	0.03
	assign (segid 3A4 and resid 402 and name N) (segid 3A4 and resid 403 and name C)	4.73	0.04	0.04
10	assign (segid 3A4 and resid 402 and name N) (segid 3A4 and resid 403 and name CA)	4.24	0.04	0.04
	assign (segid 3A4 and resid 402 and name N) (segid 3A4 and resid 403 and name CB)	5.01	0.08	0.08
	assign (segid 3A4 and resid 402 and name N) (segid 3A4 and resid 403 and name N)	2.85	0.05	0.04
	assign (segid 3A4 and resid 402 and name N) (segid 3A4 and resid 403 and name O)	5.78	0.05	0.05
	assign (segid 3A4 and resid 402 and name N) (segid 3A4 and resid 404 and name C)	5.68	0.07	0.06
15	assign (segid 3A4 and resid 402 and name N) (segid 3A4 and resid 404 and name CA)	5.40	0.10	0.11
	assign (segid 3A4 and resid 402 and name N) (segid 3A4 and resid 404 and name CB)	5.48	0.15	0.16
	assign (segid 3A4 and resid 402 and name N) (segid 3A4 and resid 404 and name N)	4.40	0.11	0.10
	assign (segid 3A4 and resid 402 and name N) (segid 3A4 and resid 404 and name O)	6.85	0.05	0.05
	assign (segid 3A4 and resid 402 and name N) (segid 3A4 and resid 405 and name C)	6.36	0.09	0.09
20	assign (segid 3A4 and resid 402 and name N) (segid 3A4 and resid 405 and name CA)	5.67	0.06	0.07
	assign (segid 3A4 and resid 402 and name N) (segid 3A4 and resid 405 and name CB)	5.21	0.13	0.12
	assign (segid 3A4 and resid 402 and name N) (segid 3A4 and resid 405 and name N)	4.89	0.07	0.08
	assign (segid 3A4 and resid 402 and name N) (segid 3A4 and resid 405 and name O)	7.54	0.13	0.14
	assign (segid 3A4 and resid 402 and name N) (segid 3A4 and resid 406 and name C)	6.98	0.19	0.18
25	assign (segid 3A4 and resid 402 and name N) (segid 3A4 and resid 406 and name CA)	5.92	0.14	0.14
	assign (segid 3A4 and resid 402 and name N) (segid 3A4 and resid 406 and name CB)	3.30	0.03	0.04
	assign (segid 3A4 and resid 402 and name O) (segid 3A4 and resid 403 and name C)	3.00	0.04	0.04
	assign (segid 3A4 and resid 402 and name O) (segid 3A4 and resid 403 and name CA)	2.76	0.03	0.03
	assign (segid 3A4 and resid 402 and name O) (segid 3A4 and resid 403 and name CB)	4.24	0.04	0.05
30	assign (segid 3A4 and resid 402 and name O) (segid 3A4 and resid 403 and name N)	2.24	0.02	0.02
	assign (segid 3A4 and resid 402 and name O) (segid 3A4 and resid 403 and name O)	3.43	0.11	0.11
	assign (segid 3A4 and resid 402 and name O) (segid 3A4 and resid 404 and name C)	4.26	0.09	0.09
	assign (segid 3A4 and resid 402 and name O) (segid 3A4 and resid 404 and name CA)	4.53	0.12	0.11
	assign (segid 3A4 and resid 402 and name O) (segid 3A4 and resid 404 and name CB)	5.52	0.12	0.12
35	assign (segid 3A4 and resid 402 and name O) (segid 3A4 and resid 404 and name N)	3.56	0.12	0.11
	assign (segid 3A4 and resid 402 and name O) (segid 3A4 and resid 404 and name O)	5.05	0.05	0.06
	assign (segid 3A4 and resid 402 and name O) (segid 3A4 and resid 405 and name C)	3.97	0.10	0.11
	assign (segid 3A4 and resid 402 and name O) (segid 3A4 and resid 405 and name CA)	4.13	0.15	0.15
	assign (segid 3A4 and resid 402 and name O) (segid 3A4 and resid 405 and name CB)	4.25	0.20	0.21
40	assign (segid 3A4 and resid 402 and name O) (segid 3A4 and resid 405 and name N)	3.66	0.18	0.17
	assign (segid 3A4 and resid 402 and name O) (segid 3A4 and resid 405 and name O)	5.10	0.10	0.11
	assign (segid 3A4 and resid 402 and name O) (segid 3A4 and resid 406 and name C)	4.79	0.12	0.13
	assign (segid 3A4 and resid 402 and name O) (segid 3A4 and resid 406 and name CA)	3.69	0.11	0.11
	assign (segid 3A4 and resid 402 and name O) (segid 3A4 and resid 406 and name N)	3.01	0.05	0.06
45	assign (segid 3A4 and resid 402 and name O) (segid 3A4 and resid 406 and name O)	5.90	0.14	0.14
	assign (segid 3A4 and resid 402 and name O) (segid 3A4 and resid 407 and name C)	7.14	0.11	0.12
	assign (segid 3A4 and resid 402 and name O) (segid 3A4 and resid 407 and name CA)	6.19	0.15	0.14
	assign (segid 3A4 and resid 402 and name O) (segid 3A4 and resid 407 and name CB)	6.41	0.17	0.17
	assign (segid 3A4 and resid 402 and name O) (segid 3A4 and resid 407 and name N)	4.85	0.15	0.14
50	assign (segid 3A4 and resid 402 and name O) (segid 3A4 and resid 408 and name N)	6.93	0.09	0.08
	assign (segid 3A4 and resid 403 and name C) (segid 3A4 and resid 403 and name CB)	2.53	0.03	0.03
	assign (segid 3A4 and resid 403 and name C) (segid 3A4 and resid 403 and name O)	1.24	0.01	0.01
	assign (segid 3A4 and resid 403 and name C) (segid 3A4 and resid 404 and name C)	3.02	0.04	0.05
	assign (segid 3A4 and resid 403 and name C) (segid 3A4 and resid 404 and name CA)	2.44	0.02	0.02
55	assign (segid 3A4 and resid 403 and name C) (segid 3A4 and resid 404 and name CB)	3.72	0.05	0.05
	assign (segid 3A4 and resid 403 and name C) (segid 3A4 and resid 404 and name N)	1.32	0.01	0.02
	assign (segid 3A4 and resid 403 and name C) (segid 3A4 and resid 404 and name O)	3.75	0.09	0.09
	assign (segid 3A4 and resid 403 and name C) (segid 3A4 and resid 405 and name C)	4.67	0.12	0.11
	assign (segid 3A4 and resid 403 and name C) (segid 3A4 and resid 405 and name CA)	4.60	0.09	0.08
60	assign (segid 3A4 and resid 403 and name C) (segid 3A4 and resid 405 and name CB)	5.46	0.13	0.13
	assign (segid 3A4 and resid 403 and name C) (segid 3A4 and resid 405 and name N)	3.43	0.08	0.08
	assign (segid 3A4 and resid 403 and name C) (segid 3A4 and resid 405 and name O)	5.71	0.15	0.16
	assign (segid 3A4 and resid 403 and name C) (segid 3A4 and resid 406 and name C)	4.94	0.07	0.06
	assign (segid 3A4 and resid 403 and name C) (segid 3A4 and resid 406 and name CA)	4.70	0.09	0.09
65	assign (segid 3A4 and resid 403 and name C) (segid 3A4 and resid 406 and name N)	3.98	0.09	0.09
	assign (segid 3A4 and resid 403 and name C) (segid 3A4 and resid 406 and name O)	6.11	0.06	0.07
	assign (segid 3A4 and resid 403 and name C) (segid 3A4 and resid 407 and name C)	6.02	0.11	0.11
	assign (segid 3A4 and resid 403 and name C) (segid 3A4 and resid 407 and name CA)	5.04	0.08	0.08
	assign (segid 3A4 and resid 403 and name C) (segid 3A4 and resid 407 and name CB)	4.59	0.09	0.09
70	assign (segid 3A4 and resid 403 and name C) (segid 3A4 and resid 407 and name N)	4.20	0.11	0.11
	assign (segid 3A4 and resid 403 and name C) (segid 3A4 and resid 407 and name O)	7.18	0.10	0.11
	assign (segid 3A4 and resid 403 and name C) (segid 3A4 and resid 408 and name CA)	7.11	0.14	0.14
	assign (segid 3A4 and resid 403 and name C) (segid 3A4 and resid 408 and name CB)	7.16	0.20	0.20
	assign (segid 3A4 and resid 403 and name C) (segid 3A4 and resid 408 and name N)	5.86	0.11	0.11
75	assign (segid 3A4 and resid 403 and name CA) (segid 3A4 and resid 403 and name C)	1.52	0.00	0.01
	assign (segid 3A4 and resid 403 and name CA) (segid 3A4 and resid 403 and name CB)	1.54	0.01	0.01
	assign (segid 3A4 and resid 403 and name CA) (segid 3A4 and resid 403 and name O)	2.40	0.01	0.01
	assign (segid 3A4 and resid 403 and name CA) (segid 3A4 and resid 404 and name C)	4.42	0.04	0.05
	assign (segid 3A4 and resid 403 and name CA) (segid 3A4 and resid 404 and name CA)	3.81	0.03	0.04
80	assign (segid 3A4 and resid 403 and name CA) (segid 3A4 and resid 404 and name CB)	4.87	0.08	0.08
	assign (segid 3A4 and resid 403 and name CA) (segid 3A4 and resid 404 and name N)	2.44	0.04	0.03
	assign (segid 3A4 and resid 403 and name CA) (segid 3A4 and resid 404 and name O)	5.22	0.09	0.09
	assign (segid 3A4 and resid 403 and name CA) (segid 3A4 and resid 405 and name C)	5.63	0.12	0.12
	assign (segid 3A4 and resid 403 and name CA) (segid 3A4 and resid 405 and name CA)	5.64	0.10	0.09
	assign (segid 3A4 and resid 403 and name CA) (segid 3A4 and resid 405 and name CB)	6.21	0.15	0.15
	assign (segid 3A4 and resid 403 and name CA) (segid 3A4 and resid 405 and name N)	4.55	0.08	0.09
	assign (segid 3A4 and resid 403 and name CA) (segid 3A4 and resid 405 and name O)	6.73	0.13	0.12

	assign (segid 3A4 and resid 403 and name CA)	(segid 3A4 and resid 406 and name C)	5.74	0.08	0.07
	assign (segid 3A4 and resid 403 and name CA)	(segid 3A4 and resid 406 and name CA)	5.27	0.11	0.11
	assign (segid 3A4 and resid 403 and name CA)	(segid 3A4 and resid 406 and name N)	4.73	0.12	0.12
	assign (segid 3A4 and resid 403 and name CA)	(segid 3A4 and resid 406 and name O)	6.88	0.13	0.13
5	assign (segid 3A4 and resid 403 and name CA)	(segid 3A4 and resid 407 and name C)	7.27	0.13	0.12
	assign (segid 3A4 and resid 403 and name CA)	(segid 3A4 and resid 407 and name CA)	6.12	0.12	0.12
	assign (segid 3A4 and resid 403 and name CA)	(segid 3A4 and resid 407 and name CB)	5.68	0.17	0.17
	assign (segid 3A4 and resid 403 and name CA)	(segid 3A4 and resid 407 and name N)	5.20	0.12	0.13
	assign (segid 3A4 and resid 403 and name CA)	(segid 3A4 and resid 408 and name CA)	8.52	0.13	0.13
10	assign (segid 3A4 and resid 403 and name CA)	(segid 3A4 and resid 408 and name CB)	8.61	0.18	0.18
	assign (segid 3A4 and resid 403 and name CA)	(segid 3A4 and resid 408 and name N)	7.22	0.12	0.12
	assign (segid 3A4 and resid 403 and name CA)	(segid 3A4 and resid 409 and name CA)	10.35	0.30	0.31
	assign (segid 3A4 and resid 403 and name CA)	(segid 3A4 and resid 409 and name CB)	10.28	0.49	0.49
	assign (segid 3A4 and resid 403 and name CA)	(segid 3A4 and resid 410 and name CA)	10.88	0.48	0.49
	assign (segid 3A4 and resid 403 and name CA)	(segid 3A4 and resid 411 and name CA)	12.41	0.35	0.36
15	assign (segid 3A4 and resid 403 and name CA)	(segid 3A4 and resid 411 and name CB)	11.85	0.40	0.40
	assign (segid 3A4 and resid 403 and name CA)	(segid 3A4 and resid 412 and name CA)	14.30	0.39	0.40
	assign (segid 3A4 and resid 403 and name CA)	(segid 3A4 and resid 413 and name CA)	17.84	0.77	0.78
	assign (segid 3A4 and resid 403 and name CA)	(segid 3A4 and resid 414 and name CA)	17.70	0.97	0.96
20	assign (segid 3A4 and resid 403 and name CB)	(segid 3A4 and resid 404 and name C)	5.44	0.06	0.06
	assign (segid 3A4 and resid 403 and name CB)	(segid 3A4 and resid 404 and name CA)	4.48	0.08	0.08
	assign (segid 3A4 and resid 403 and name CB)	(segid 3A4 and resid 404 and name CB)	5.35	0.17	0.16
	assign (segid 3A4 and resid 403 and name CB)	(segid 3A4 and resid 404 and name N)	3.15	0.08	0.08
	assign (segid 3A4 and resid 403 and name CB)	(segid 3A4 and resid 404 and name O)	6.21	0.10	0.10
25	assign (segid 3A4 and resid 403 and name CB)	(segid 3A4 and resid 405 and name C)	7.06	0.11	0.11
	assign (segid 3A4 and resid 403 and name CB)	(segid 3A4 and resid 405 and name CA)	6.98	0.07	0.07
	assign (segid 3A4 and resid 403 and name CB)	(segid 3A4 and resid 405 and name CB)	7.60	0.13	0.12
	assign (segid 3A4 and resid 403 and name CB)	(segid 3A4 and resid 405 and name N)	5.77	0.07	0.06
	assign (segid 3A4 and resid 403 and name CB)	(segid 3A4 and resid 406 and name C)	6.99	0.11	0.10
30	assign (segid 3A4 and resid 403 and name CB)	(segid 3A4 and resid 406 and name CA)	6.68	0.12	0.13
	assign (segid 3A4 and resid 403 and name CB)	(segid 3A4 and resid 406 and name N)	6.20	0.13	0.12
	assign (segid 3A4 and resid 403 and name CB)	(segid 3A4 and resid 407 and name CA)	6.99	0.14	0.15
	assign (segid 3A4 and resid 403 and name CB)	(segid 3A4 and resid 407 and name CB)	6.26	0.20	0.20
	assign (segid 3A4 and resid 403 and name CB)	(segid 3A4 and resid 407 and name N)	6.30	0.14	0.15
35	assign (segid 3A4 and resid 403 and name CB)	(segid 3A4 and resid 408 and name CA)	9.47	0.17	0.18
	assign (segid 3A4 and resid 403 and name CB)	(segid 3A4 and resid 408 and name CB)	9.59	0.21	0.21
	assign (segid 3A4 and resid 403 and name CB)	(segid 3A4 and resid 409 and name CA)	11.62	0.27	0.26
	assign (segid 3A4 and resid 403 and name CB)	(segid 3A4 and resid 409 and name CB)	11.65	0.44	0.43
	assign (segid 3A4 and resid 403 and name CB)	(segid 3A4 and resid 410 and name CA)	11.97	0.51	0.51
40	assign (segid 3A4 and resid 403 and name CB)	(segid 3A4 and resid 411 and name CA)	13.24	0.43	0.43
	assign (segid 3A4 and resid 403 and name CB)	(segid 3A4 and resid 411 and name CB)	12.55	0.48	0.48
	assign (segid 3A4 and resid 403 and name CB)	(segid 3A4 and resid 412 and name CA)	15.29	0.47	0.47
	assign (segid 3A4 and resid 403 and name N)	(segid 3A4 and resid 403 and name C)	2.46	0.01	0.01
	assign (segid 3A4 and resid 403 and name N)	(segid 3A4 and resid 403 and name CA)	1.46	0.01	0.00
45	assign (segid 3A4 and resid 403 and name N)	(segid 3A4 and resid 403 and name CB)	2.45	0.03	0.03
	assign (segid 3A4 and resid 403 and name N)	(segid 3A4 and resid 403 and name O)	3.48	0.03	0.04
	assign (segid 3A4 and resid 403 and name N)	(segid 3A4 and resid 404 and name C)	4.73	0.06	0.06
	assign (segid 3A4 and resid 403 and name N)	(segid 3A4 and resid 404 and name CA)	4.24	0.06	0.06
	assign (segid 3A4 and resid 403 and name N)	(segid 3A4 and resid 404 and name CB)	5.00	0.09	0.09
50	assign (segid 3A4 and resid 403 and name N)	(segid 3A4 and resid 404 and name N)	2.84	0.06	0.05
	assign (segid 3A4 and resid 403 and name N)	(segid 3A4 and resid 404 and name O)	5.72	0.07	0.08
	assign (segid 3A4 and resid 403 and name N)	(segid 3A4 and resid 405 and name C)	5.69	0.09	0.09
	assign (segid 3A4 and resid 403 and name N)	(segid 3A4 and resid 405 and name CA)	5.49	0.10	0.11
	assign (segid 3A4 and resid 403 and name N)	(segid 3A4 and resid 405 and name CB)	5.72	0.15	0.14
55	assign (segid 3A4 and resid 403 and name N)	(segid 3A4 and resid 405 and name N)	4.48	0.10	0.11
	assign (segid 3A4 and resid 403 and name N)	(segid 3A4 and resid 405 and name O)	6.87	0.08	0.08
	assign (segid 3A4 and resid 403 and name N)	(segid 3A4 and resid 406 and name C)	6.38	0.07	0.06
	assign (segid 3A4 and resid 403 and name N)	(segid 3A4 and resid 406 and name CA)	5.59	0.07	0.08
	assign (segid 3A4 and resid 403 and name N)	(segid 3A4 and resid 406 and name N)	4.86	0.08	0.08
60	assign (segid 3A4 and resid 403 and name N)	(segid 3A4 and resid 406 and name O)	7.54	0.11	0.12
	assign (segid 3A4 and resid 403 and name N)	(segid 3A4 and resid 407 and name CA)	7.13	0.09	0.09
	assign (segid 3A4 and resid 403 and name N)	(segid 3A4 and resid 407 and name CB)	6.87	0.13	0.13
	assign (segid 3A4 and resid 403 and name N)	(segid 3A4 and resid 407 and name N)	6.04	0.10	0.10
	assign (segid 3A4 and resid 403 and name O)	(segid 3A4 and resid 403 and name CB)	3.34	0.04	0.04
65	assign (segid 3A4 and resid 403 and name O)	(segid 3A4 and resid 404 and name C)	2.97	0.08	0.07
	assign (segid 3A4 and resid 403 and name O)	(segid 3A4 and resid 404 and name CA)	2.77	0.02	0.02
	assign (segid 3A4 and resid 403 and name O)	(segid 3A4 and resid 404 and name CB)	4.27	0.05	0.04
	assign (segid 3A4 and resid 403 and name O)	(segid 3A4 and resid 404 and name N)	2.25	0.02	0.01
	assign (segid 3A4 and resid 403 and name O)	(segid 3A4 and resid 404 and name O)	3.30	0.14	0.13
70	assign (segid 3A4 and resid 403 and name O)	(segid 3A4 and resid 405 and name C)	4.28	0.14	0.14
	assign (segid 3A4 and resid 403 and name O)	(segid 3A4 and resid 405 and name CA)	4.54	0.09	0.08
	assign (segid 3A4 and resid 403 and name O)	(segid 3A4 and resid 405 and name CB)	5.61	0.15	0.15
	assign (segid 3A4 and resid 403 and name O)	(segid 3A4 and resid 405 and name N)	3.60	0.07	0.06
	assign (segid 3A4 and resid 403 and name O)	(segid 3A4 and resid 405 and name O)	5.16	0.22	0.23
75	assign (segid 3A4 and resid 403 and name O)	(segid 3A4 and resid 406 and name C)	3.95	0.09	0.09
	assign (segid 3A4 and resid 403 and name O)	(segid 3A4 and resid 406 and name CA)	4.01	0.11	0.12
	assign (segid 3A4 and resid 403 and name O)	(segid 3A4 and resid 406 and name N)	3.55	0.09	0.08
	assign (segid 3A4 and resid 403 and name O)	(segid 3A4 and resid 406 and name O)	5.08	0.08	0.08
	assign (segid 3A4 and resid 403 and name O)	(segid 3A4 and resid 407 and name C)	4.91	0.13	0.13
80	assign (segid 3A4 and resid 403 and name O)	(segid 3A4 and resid 407 and name CA)	3.84	0.10	0.09
	assign (segid 3A4 and resid 403 and name O)	(segid 3A4 and resid 407 and name CB)	3.42	0.12	0.11
	assign (segid 3A4 and resid 403 and name O)	(segid 3A4 and resid 407 and name N)	3.08	0.13	0.14
	assign (segid 3A4 and resid 403 and name O)	(segid 3A4 and resid 407 and name O)	6.04	0.12	0.12

	assign (segid 3A4 and resid 403 and name O) (segid 3A4 and resid 408 and name C)	7.24	0.14	0.14
	assign (segid 3A4 and resid 403 and name O) (segid 3A4 and resid 408 and name CA)	6.24	0.14	0.15
	assign (segid 3A4 and resid 403 and name O) (segid 3A4 and resid 408 and name CB)	6.51	0.18	0.18
	assign (segid 3A4 and resid 403 and name O) (segid 3A4 and resid 408 and name N)	4.91	0.13	0.13
5	assign (segid 3A4 and resid 403 and name O) (segid 3A4 and resid 409 and name N)	7.15	0.22	0.21
	assign (segid 3A4 and resid 404 and name C) (segid 3A4 and resid 404 and name CB)	2.49	0.02	0.03
	assign (segid 3A4 and resid 404 and name C) (segid 3A4 and resid 404 and name O)	1.23	0.01	0.01
	assign (segid 3A4 and resid 404 and name C) (segid 3A4 and resid 405 and name C)	3.05	0.10	0.09
	assign (segid 3A4 and resid 404 and name C) (segid 3A4 and resid 405 and name CA)	2.43	0.02	0.02
10	assign (segid 3A4 and resid 404 and name C) (segid 3A4 and resid 405 and name CB)	3.69	0.02	0.03
	assign (segid 3A4 and resid 404 and name C) (segid 3A4 and resid 405 and name N)	1.33	0.01	0.01
	assign (segid 3A4 and resid 404 and name C) (segid 3A4 and resid 405 and name O)	3.88	0.20	0.20
	assign (segid 3A4 and resid 404 and name C) (segid 3A4 and resid 406 and name C)	4.58	0.09	0.10
	assign (segid 3A4 and resid 404 and name C) (segid 3A4 and resid 406 and name CA)	4.51	0.07	0.07
	assign (segid 3A4 and resid 404 and name C) (segid 3A4 and resid 406 and name N)	3.32	0.02	0.02
15	assign (segid 3A4 and resid 404 and name C) (segid 3A4 and resid 406 and name O)	5.66	0.14	0.14
	assign (segid 3A4 and resid 404 and name C) (segid 3A4 and resid 407 and name C)	4.84	0.03	0.04
	assign (segid 3A4 and resid 404 and name C) (segid 3A4 and resid 407 and name CA)	4.62	0.06	0.06
	assign (segid 3A4 and resid 404 and name C) (segid 3A4 and resid 407 and name CB)	4.62	0.15	0.14
20	assign (segid 3A4 and resid 404 and name C) (segid 3A4 and resid 407 and name N)	3.87	0.08	0.08
	assign (segid 3A4 and resid 404 and name C) (segid 3A4 and resid 407 and name O)	6.05	0.03	0.03
	assign (segid 3A4 and resid 404 and name C) (segid 3A4 and resid 408 and name C)	6.03	0.12	0.12
	assign (segid 3A4 and resid 404 and name C) (segid 3A4 and resid 408 and name CA)	4.92	0.09	0.09
	assign (segid 3A4 and resid 404 and name C) (segid 3A4 and resid 408 and name CB)	4.52	0.18	0.18
25	assign (segid 3A4 and resid 404 and name C) (segid 3A4 and resid 408 and name N)	4.06	0.03	0.03
	assign (segid 3A4 and resid 404 and name C) (segid 3A4 and resid 408 and name O)	7.18	0.10	0.10
	assign (segid 3A4 and resid 404 and name C) (segid 3A4 and resid 409 and name CA)	7.24	0.23	0.22
	assign (segid 3A4 and resid 404 and name C) (segid 3A4 and resid 409 and name CG)	7.08	0.35	0.36
	assign (segid 3A4 and resid 404 and name C) (segid 3A4 and resid 409 and name N)	5.95	0.19	0.18
30	assign (segid 3A4 and resid 404 and name C) (segid 3A4 and resid 404 and name C)	1.53	0.01	0.00
	assign (segid 3A4 and resid 404 and name CA) (segid 3A4 and resid 404 and name CB)	1.54	0.03	0.02
	assign (segid 3A4 and resid 404 and name CA) (segid 3A4 and resid 404 and name O)	2.38	0.01	0.02
	assign (segid 3A4 and resid 404 and name CA) (segid 3A4 and resid 405 and name C)	4.46	0.09	0.08
	assign (segid 3A4 and resid 404 and name CA) (segid 3A4 and resid 405 and name CA)	3.80	0.02	0.03
35	assign (segid 3A4 and resid 404 and name CA) (segid 3A4 and resid 405 and name CB)	4.85	0.04	0.04
	assign (segid 3A4 and resid 404 and name CA) (segid 3A4 and resid 405 and name N)	2.44	0.02	0.02
	assign (segid 3A4 and resid 404 and name CA) (segid 3A4 and resid 405 and name O)	5.36	0.19	0.18
	assign (segid 3A4 and resid 404 and name CA) (segid 3A4 and resid 406 and name C)	5.60	0.08	0.09
	assign (segid 3A4 and resid 404 and name CA) (segid 3A4 and resid 406 and name CA)	5.56	0.07	0.07
40	assign (segid 3A4 and resid 404 and name CA) (segid 3A4 and resid 406 and name N)	4.46	0.03	0.03
	assign (segid 3A4 and resid 404 and name CA) (segid 3A4 and resid 406 and name O)	6.72	0.09	0.09
	assign (segid 3A4 and resid 404 and name CA) (segid 3A4 and resid 407 and name C)	5.70	0.06	0.07
	assign (segid 3A4 and resid 404 and name CA) (segid 3A4 and resid 407 and name CA)	5.30	0.06	0.06
	assign (segid 3A4 and resid 404 and name CA) (segid 3A4 and resid 407 and name CB)	4.86	0.12	0.11
45	assign (segid 3A4 and resid 404 and name CA) (segid 3A4 and resid 407 and name N)	4.71	0.09	0.08
	assign (segid 3A4 and resid 404 and name CA) (segid 3A4 and resid 407 and name O)	6.88	0.08	0.07
	assign (segid 3A4 and resid 404 and name CA) (segid 3A4 and resid 408 and name C)	7.23	0.13	0.14
	assign (segid 3A4 and resid 404 and name CA) (segid 3A4 and resid 408 and name CA)	5.98	0.16	0.17
	assign (segid 3A4 and resid 404 and name CA) (segid 3A4 and resid 408 and name CB)	5.62	0.25	0.25
50	assign (segid 3A4 and resid 404 and name CA) (segid 3A4 and resid 408 and name N)	5.09	0.10	0.09
	assign (segid 3A4 and resid 404 and name CA) (segid 3A4 and resid 409 and name CA)	8.63	0.19	0.19
	assign (segid 3A4 and resid 404 and name CA) (segid 3A4 and resid 409 and name CB)	8.80	0.27	0.27
	assign (segid 3A4 and resid 404 and name CA) (segid 3A4 and resid 409 and name N)	7.30	0.17	0.16
	assign (segid 3A4 and resid 404 and name CA) (segid 3A4 and resid 410 and name CA)	10.06	0.33	0.34
55	assign (segid 3A4 and resid 404 and name CA) (segid 3A4 and resid 411 and name CA)	10.79	0.24	0.23
	assign (segid 3A4 and resid 404 and name CA) (segid 3A4 and resid 411 and name CB)	10.07	0.32	0.31
	assign (segid 3A4 and resid 404 and name CA) (segid 3A4 and resid 412 and name CA)	12.00	0.42	0.41
	assign (segid 3A4 and resid 404 and name CA) (segid 3A4 and resid 413 and name CA)	15.35	0.73	0.73
	assign (segid 3A4 and resid 404 and name CA) (segid 3A4 and resid 414 and name CA)	14.75	0.81	0.81
60	assign (segid 3A4 and resid 404 and name CA) (segid 3A4 and resid 415 and name CA)	17.22	0.85	0.84
	assign (segid 3A4 and resid 404 and name CA) (segid 3A4 and resid 415 and name CB)	18.30	0.77	0.77
	assign (segid 3A4 and resid 404 and name CA) (segid 3A4 and resid 434 and name CA)	17.78	0.78	0.78
	assign (segid 3A4 and resid 404 and name CA) (segid 3A4 and resid 435 and name CA)	17.41	0.62	0.62
	assign (segid 3A4 and resid 404 and name CA) (segid 3A4 and resid 438 and name CA)	16.79	1.05	1.06
65	assign (segid 3A4 and resid 404 and name CA) (segid 3A4 and resid 439 and name CA)	17.70	0.59	0.59
	assign (segid 3A4 and resid 404 and name CA) (segid 3A4 and resid 440 and name CA)	16.14	0.62	0.63
	assign (segid 3A4 and resid 404 and name CB) (segid 3A4 and resid 405 and name C)	5.39	0.10	0.10
	assign (segid 3A4 and resid 404 and name CB) (segid 3A4 and resid 405 and name CA)	4.37	0.08	0.08
	assign (segid 3A4 and resid 404 and name CB) (segid 3A4 and resid 405 and name CB)	5.16	0.12	0.13
70	assign (segid 3A4 and resid 404 and name CB) (segid 3A4 and resid 405 and name N)	3.04	0.07	0.08
	assign (segid 3A4 and resid 404 and name CB) (segid 3A4 and resid 405 and name O)	6.25	0.18	0.19
	assign (segid 3A4 and resid 404 and name CB) (segid 3A4 and resid 406 and name C)	6.98	0.10	0.11
	assign (segid 3A4 and resid 404 and name CB) (segid 3A4 and resid 406 and name CA)	6.86	0.09	0.08
	assign (segid 3A4 and resid 404 and name CB) (segid 3A4 and resid 406 and name N)	5.61	0.04	0.05
75	assign (segid 3A4 and resid 404 and name CB) (segid 3A4 and resid 407 and name C)	6.90	0.06	0.05
	assign (segid 3A4 and resid 404 and name CB) (segid 3A4 and resid 407 and name CA)	6.68	0.08	0.08
	assign (segid 3A4 and resid 404 and name CB) (segid 3A4 and resid 407 and name CB)	6.22	0.16	0.17
	assign (segid 3A4 and resid 404 and name CB) (segid 3A4 and resid 407 and name N)	6.14	0.10	0.10
	assign (segid 3A4 and resid 404 and name CB) (segid 3A4 and resid 408 and name CA)	6.74	0.16	0.16
80	assign (segid 3A4 and resid 404 and name CB) (segid 3A4 and resid 408 and name CB)	6.07	0.26	0.27
	assign (segid 3A4 and resid 404 and name CB) (segid 3A4 and resid 408 and name N)	6.10	0.07	0.07
	assign (segid 3A4 and resid 404 and name CB) (segid 3A4 and resid 409 and name CA)	9.47	0.21	0.21
	assign (segid 3A4 and resid 404 and name CB) (segid 3A4 and resid 409 and name CB)	9.61	0.26	0.25

	assign (segid 3A4 and resid 404 and name CB)	(segid 3A4 and resid 410 and name CA)	11.26	0.27	0.26
	assign (segid 3A4 and resid 404 and name CB)	(segid 3A4 and resid 411 and name CA)	11.77	0.18	0.18
	assign (segid 3A4 and resid 404 and name CB)	(segid 3A4 and resid 411 and name CB)	11.00	0.29	0.29
	assign (segid 3A4 and resid 404 and name CB)	(segid 3A4 and resid 412 and name CA)	12.64	0.41	0.41
5	assign (segid 3A4 and resid 404 and name CB)	(segid 3A4 and resid 413 and name CA)	15.71	0.76	0.77
	assign (segid 3A4 and resid 404 and name CB)	(segid 3A4 and resid 414 and name CA)	14.79	0.64	0.64
	assign (segid 3A4 and resid 404 and name CB)	(segid 3A4 and resid 415 and name CA)	17.01	0.84	0.85
	assign (segid 3A4 and resid 404 and name CB)	(segid 3A4 and resid 415 and name CB)	18.12	0.83	0.83
	assign (segid 3A4 and resid 404 and name CB)	(segid 3A4 and resid 416 and name CA)	18.21	1.08	1.07
10	assign (segid 3A4 and resid 404 and name CB)	(segid 3A4 and resid 433 and name CA)	18.56	0.54	0.55
	assign (segid 3A4 and resid 404 and name CB)	(segid 3A4 and resid 434 and name CA)	16.38	0.78	0.78
	assign (segid 3A4 and resid 404 and name CB)	(segid 3A4 and resid 435 and name CA)	16.10	0.68	0.68
	assign (segid 3A4 and resid 404 and name CB)	(segid 3A4 and resid 436 and name CA)	17.80	1.12	1.12
	assign (segid 3A4 and resid 404 and name CB)	(segid 3A4 and resid 437 and name CA)	17.45	1.10	1.11
15	assign (segid 3A4 and resid 404 and name CB)	(segid 3A4 and resid 438 and name CA)	15.79	1.11	1.11
	assign (segid 3A4 and resid 404 and name CB)	(segid 3A4 and resid 439 and name CA)	16.91	0.55	0.56
	assign (segid 3A4 and resid 404 and name CB)	(segid 3A4 and resid 440 and name CA)	15.65	0.61	0.60
	assign (segid 3A4 and resid 404 and name N)	(segid 3A4 and resid 404 and name C)	2.46	0.04	0.03
	assign (segid 3A4 and resid 404 and name N)	(segid 3A4 and resid 404 and name CA)	1.46	0.01	0.01
20	assign (segid 3A4 and resid 404 and name N)	(segid 3A4 and resid 404 and name CB)	2.46	0.05	0.06
	assign (segid 3A4 and resid 404 and name N)	(segid 3A4 and resid 404 and name O)	3.44	0.05	0.04
	assign (segid 3A4 and resid 404 and name N)	(segid 3A4 and resid 405 and name C)	4.76	0.09	0.09
	assign (segid 3A4 and resid 404 and name N)	(segid 3A4 and resid 405 and name CA)	4.27	0.06	0.07
	assign (segid 3A4 and resid 404 and name N)	(segid 3A4 and resid 405 and name CB)	5.08	0.07	0.08
25	assign (segid 3A4 and resid 404 and name N)	(segid 3A4 and resid 405 and name N)	2.89	0.06	0.06
	assign (segid 3A4 and resid 404 and name N)	(segid 3A4 and resid 405 and name O)	5.83	0.14	0.13
	assign (segid 3A4 and resid 404 and name N)	(segid 3A4 and resid 406 and name C)	5.67	0.05	0.06
	assign (segid 3A4 and resid 404 and name N)	(segid 3A4 and resid 406 and name CA)	5.41	0.07	0.07
	assign (segid 3A4 and resid 404 and name N)	(segid 3A4 and resid 406 and name N)	4.40	0.07	0.06
30	assign (segid 3A4 and resid 404 and name N)	(segid 3A4 and resid 406 and name O)	6.86	0.03	0.04
	assign (segid 3A4 and resid 404 and name N)	(segid 3A4 and resid 407 and name C)	6.41	0.09	0.08
	assign (segid 3A4 and resid 404 and name N)	(segid 3A4 and resid 407 and name CA)	5.68	0.06	0.06
	assign (segid 3A4 and resid 404 and name N)	(segid 3A4 and resid 407 and name CB)	5.21	0.04	0.04
	assign (segid 3A4 and resid 404 and name N)	(segid 3A4 and resid 407 and name N)	4.90	0.08	0.08
35	assign (segid 3A4 and resid 404 and name N)	(segid 3A4 and resid 407 and name O)	7.60	0.09	0.08
	assign (segid 3A4 and resid 404 and name N)	(segid 3A4 and resid 408 and name CA)	7.06	0.15	0.15
	assign (segid 3A4 and resid 404 and name N)	(segid 3A4 and resid 408 and name CB)	6.85	0.23	0.22
	assign (segid 3A4 and resid 404 and name N)	(segid 3A4 and resid 408 and name N)	5.99	0.10	0.10
	assign (segid 3A4 and resid 404 and name N)	(segid 3A4 and resid 408 and name CB)	3.35	0.04	0.03
40	assign (segid 3A4 and resid 404 and name O)	(segid 3A4 and resid 405 and name C)	3.01	0.13	0.12
	assign (segid 3A4 and resid 404 and name O)	(segid 3A4 and resid 405 and name CA)	2.77	0.02	0.02
	assign (segid 3A4 and resid 404 and name O)	(segid 3A4 and resid 405 and name CB)	4.24	0.05	0.04
	assign (segid 3A4 and resid 404 and name O)	(segid 3A4 and resid 405 and name N)	2.25	0.00	0.01
	assign (segid 3A4 and resid 404 and name O)	(segid 3A4 and resid 406 and name C)	3.49	0.28	0.28
45	assign (segid 3A4 and resid 404 and name O)	(segid 3A4 and resid 406 and name CA)	4.10	0.17	0.16
	assign (segid 3A4 and resid 404 and name O)	(segid 3A4 and resid 406 and name N)	4.39	0.13	0.13
	assign (segid 3A4 and resid 404 and name O)	(segid 3A4 and resid 406 and name O)	3.44	0.08	0.08
	assign (segid 3A4 and resid 404 and name O)	(segid 3A4 and resid 406 and name O)	5.03	0.21	0.20
	assign (segid 3A4 and resid 404 and name O)	(segid 3A4 and resid 407 and name C)	3.75	0.07	0.08
50	assign (segid 3A4 and resid 404 and name O)	(segid 3A4 and resid 407 and name CA)	3.78	0.16	0.15
	assign (segid 3A4 and resid 404 and name O)	(segid 3A4 and resid 407 and name CB)	3.89	0.26	0.26
	assign (segid 3A4 and resid 404 and name O)	(segid 3A4 and resid 407 and name N)	3.28	0.18	0.18
	assign (segid 3A4 and resid 404 and name O)	(segid 3A4 and resid 407 and name O)	4.93	0.08	0.07
	assign (segid 3A4 and resid 404 and name O)	(segid 3A4 and resid 408 and name C)	4.90	0.12	0.13
55	assign (segid 3A4 and resid 404 and name O)	(segid 3A4 and resid 408 and name CA)	3.74	0.12	0.11
	assign (segid 3A4 and resid 404 and name O)	(segid 3A4 and resid 408 and name CB)	3.47	0.24	0.25
	assign (segid 3A4 and resid 404 and name O)	(segid 3A4 and resid 408 and name N)	2.89	0.02	0.02
	assign (segid 3A4 and resid 404 and name O)	(segid 3A4 and resid 408 and name O)	6.02	0.11	0.12
	assign (segid 3A4 and resid 404 and name O)	(segid 3A4 and resid 409 and name C)	7.20	0.16	0.16
60	assign (segid 3A4 and resid 404 and name O)	(segid 3A4 and resid 409 and name CA)	6.31	0.18	0.19
	assign (segid 3A4 and resid 404 and name O)	(segid 3A4 and resid 409 and name CB)	6.60	0.24	0.24
	assign (segid 3A4 and resid 404 and name O)	(segid 3A4 and resid 409 and name CG)	6.47	0.28	0.28
	assign (segid 3A4 and resid 404 and name O)	(segid 3A4 and resid 409 and name N)	4.95	0.17	0.16
	assign (segid 3A4 and resid 404 and name O)	(segid 3A4 and resid 410 and name N)	6.84	0.23	0.24
65	assign (segid 3A4 and resid 405 and name C)	(segid 3A4 and resid 405 and name CB)	2.50	0.05	0.05
	assign (segid 3A4 and resid 405 and name C)	(segid 3A4 and resid 405 and name O)	1.24	0.01	0.01
	assign (segid 3A4 and resid 405 and name C)	(segid 3A4 and resid 406 and name C)	3.03	0.12	0.12
	assign (segid 3A4 and resid 405 and name C)	(segid 3A4 and resid 406 and name CA)	2.43	0.02	0.02
	assign (segid 3A4 and resid 405 and name C)	(segid 3A4 and resid 406 and name N)	1.32	0.01	0.01
70	assign (segid 3A4 and resid 405 and name C)	(segid 3A4 and resid 406 and name O)	3.89	0.21	0.21
	assign (segid 3A4 and resid 405 and name C)	(segid 3A4 and resid 407 and name C)	4.65	0.19	0.18
	assign (segid 3A4 and resid 405 and name C)	(segid 3A4 and resid 407 and name CA)	4.50	0.10	0.09
	assign (segid 3A4 and resid 405 and name C)	(segid 3A4 and resid 407 and name CB)	5.38	0.12	0.11
	assign (segid 3A4 and resid 405 and name C)	(segid 3A4 and resid 407 and name N)	3.30	0.05	0.04
75	assign (segid 3A4 and resid 405 and name C)	(segid 3A4 and resid 407 and name O)	5.75	0.20	0.19
	assign (segid 3A4 and resid 405 and name C)	(segid 3A4 and resid 408 and name C)	5.18	0.39	0.39
	assign (segid 3A4 and resid 405 and name C)	(segid 3A4 and resid 408 and name CA)	4.81	0.28	0.28
	assign (segid 3A4 and resid 405 and name C)	(segid 3A4 and resid 408 and name CB)	4.68	0.26	0.26
	assign (segid 3A4 and resid 405 and name C)	(segid 3A4 and resid 408 and name N)	3.99	0.24	0.25
80	assign (segid 3A4 and resid 405 and name C)	(segid 3A4 and resid 408 and name O)	6.40	0.40	0.39
	assign (segid 3A4 and resid 405 and name C)	(segid 3A4 and resid 409 and name C)	6.29	0.42	0.42
	assign (segid 3A4 and resid 405 and name C)	(segid 3A4 and resid 409 and name CA)	5.37	0.49	0.49
	assign (segid 3A4 and resid 405 and name C)	(segid 3A4 and resid 409 and name CB)	5.02	0.56	0.57

	assign (segid 3A4 and resid 405 and name C) (segid 3A4 and resid 409 and name CD2)	6.14	0.65	0.65
	assign (segid 3A4 and resid 405 and name C) (segid 3A4 and resid 409 and name CG)	4.87	0.62	0.63
	assign (segid 3A4 and resid 405 and name C) (segid 3A4 and resid 409 and name N)	4.47	0.45	0.44
	assign (segid 3A4 and resid 405 and name C) (segid 3A4 and resid 410 and name N)	6.09	0.38	0.39
5	assign (segid 3A4 and resid 405 and name CA) (segid 3A4 and resid 405 and name C)	1.51	0.01	0.02
	assign (segid 3A4 and resid 405 and name CA) (segid 3A4 and resid 405 and name CB)	1.53	0.02	0.01
	assign (segid 3A4 and resid 405 and name CA) (segid 3A4 and resid 405 and name O)	2.38	0.03	0.02
	assign (segid 3A4 and resid 405 and name CA) (segid 3A4 and resid 406 and name C)	4.40	0.07	0.07
	assign (segid 3A4 and resid 405 and name CA) (segid 3A4 and resid 406 and name CA)	3.80	0.02	0.03
10	assign (segid 3A4 and resid 405 and name CA) (segid 3A4 and resid 406 and name N)	2.44	0.03	0.02
	assign (segid 3A4 and resid 405 and name CA) (segid 3A4 and resid 406 and name O)	5.32	0.17	0.17
	assign (segid 3A4 and resid 405 and name CA) (segid 3A4 and resid 407 and name C)	5.50	0.12	0.11
	assign (segid 3A4 and resid 405 and name CA) (segid 3A4 and resid 407 and name CA)	5.45	0.08	0.08
	assign (segid 3A4 and resid 405 and name CA) (segid 3A4 and resid 407 and name CB)	6.05	0.15	0.15
15	assign (segid 3A4 and resid 405 and name CA) (segid 3A4 and resid 407 and name N)	4.37	0.07	0.07
	assign (segid 3A4 and resid 405 and name CA) (segid 3A4 and resid 407 and name O)	6.64	0.14	0.13
	assign (segid 3A4 and resid 405 and name CA) (segid 3A4 and resid 408 and name C)	5.80	0.28	0.28
	assign (segid 3A4 and resid 405 and name CA) (segid 3A4 and resid 408 and name CA)	5.21	0.19	0.19
	assign (segid 3A4 and resid 405 and name CA) (segid 3A4 and resid 408 and name CB)	4.66	0.21	0.20
20	assign (segid 3A4 and resid 405 and name CA) (segid 3A4 and resid 408 and name N)	4.60	0.15	0.15
	assign (segid 3A4 and resid 405 and name CA) (segid 3A4 and resid 408 and name O)	7.02	0.27	0.28
	assign (segid 3A4 and resid 405 and name CA) (segid 3A4 and resid 409 and name CA)	6.24	0.40	0.41
	assign (segid 3A4 and resid 405 and name CA) (segid 3A4 and resid 409 and name CB)	5.90	0.47	0.47
	assign (segid 3A4 and resid 405 and name CA) (segid 3A4 and resid 409 and name CD2)	6.47	0.66	0.66
25	assign (segid 3A4 and resid 405 and name CA) (segid 3A4 and resid 409 and name CG)	5.41	0.57	0.57
	assign (segid 3A4 and resid 405 and name CA) (segid 3A4 and resid 409 and name N)	5.26	0.35	0.34
	assign (segid 3A4 and resid 405 and name CA) (segid 3A4 and resid 410 and name CA)	8.52	0.22	0.22
	assign (segid 3A4 and resid 405 and name CA) (segid 3A4 and resid 410 and name N)	7.27	0.25	0.25
	assign (segid 3A4 and resid 405 and name CA) (segid 3A4 and resid 411 and name CA)	10.09	0.22	0.21
30	assign (segid 3A4 and resid 405 and name CA) (segid 3A4 and resid 411 and name CB)	9.86	0.33	0.33
	assign (segid 3A4 and resid 405 and name CA) (segid 3A4 and resid 412 and name CA)	10.60	0.23	0.24
	assign (segid 3A4 and resid 405 and name CA) (segid 3A4 and resid 413 and name CA)	13.22	0.68	0.68
	assign (segid 3A4 and resid 405 and name CA) (segid 3A4 and resid 414 and name CA)	12.70	0.95	0.95
	assign (segid 3A4 and resid 405 and name CA) (segid 3A4 and resid 415 and name CA)	15.19	0.87	0.88
35	assign (segid 3A4 and resid 405 and name CA) (segid 3A4 and resid 415 and name CB)	16.26	0.71	0.71
	assign (segid 3A4 and resid 405 and name CA) (segid 3A4 and resid 416 and name CA)	16.86	1.30	1.29
	assign (segid 3A4 and resid 405 and name CA) (segid 3A4 and resid 434 and name CA)	17.55	0.81	0.81
	assign (segid 3A4 and resid 405 and name CA) (segid 3A4 and resid 435 and name CA)	16.94	0.59	0.59
	assign (segid 3A4 and resid 405 and name CA) (segid 3A4 and resid 437 and name CA)	18.47	0.59	0.59
40	assign (segid 3A4 and resid 405 and name CA) (segid 3A4 and resid 438 and name CA)	16.13	0.63	0.63
	assign (segid 3A4 and resid 405 and name CA) (segid 3A4 and resid 439 and name CA)	17.03	0.65	0.64
	assign (segid 3A4 and resid 405 and name CA) (segid 3A4 and resid 440 and name CA)	15.09	0.57	0.56
	assign (segid 3A4 and resid 405 and name CB) (segid 3A4 and resid 406 and name C)	5.45	0.17	0.17
	assign (segid 3A4 and resid 405 and name CB) (segid 3A4 and resid 406 and name CA)	4.52	0.17	0.17
45	assign (segid 3A4 and resid 405 and name CB) (segid 3A4 and resid 406 and name N)	3.20	0.18	0.18
	assign (segid 3A4 and resid 405 and name CB) (segid 3A4 and resid 406 and name O)	6.33	0.27	0.26
	assign (segid 3A4 and resid 405 and name CB) (segid 3A4 and resid 407 and name C)	6.91	0.13	0.13
	assign (segid 3A4 and resid 405 and name CB) (segid 3A4 and resid 407 and name CA)	6.83	0.08	0.08
	assign (segid 3A4 and resid 405 and name CB) (segid 3A4 and resid 407 and name CB)	7.47	0.11	0.11
50	assign (segid 3A4 and resid 405 and name CB) (segid 3A4 and resid 407 and name N)	5.64	0.07	0.06
	assign (segid 3A4 and resid 405 and name CB) (segid 3A4 and resid 408 and name C)	6.96	0.32	0.33
	assign (segid 3A4 and resid 405 and name CB) (segid 3A4 and resid 408 and name CA)	6.54	0.23	0.24
	assign (segid 3A4 and resid 405 and name CB) (segid 3A4 and resid 408 and name CB)	5.88	0.27	0.26
	assign (segid 3A4 and resid 405 and name CB) (segid 3A4 and resid 408 and name N)	6.02	0.17	0.18
55	assign (segid 3A4 and resid 405 and name CB) (segid 3A4 and resid 409 and name CA)	7.01	0.49	0.50
	assign (segid 3A4 and resid 405 and name CB) (segid 3A4 and resid 409 and name CB)	6.37	0.56	0.57
	assign (segid 3A4 and resid 405 and name CB) (segid 3A4 and resid 409 and name CG)	5.67	0.70	0.70
	assign (segid 3A4 and resid 405 and name CB) (segid 3A4 and resid 409 and name N)	6.26	0.41	0.40
	assign (segid 3A4 and resid 405 and name CB) (segid 3A4 and resid 410 and name CA)	9.48	0.30	0.31
60	assign (segid 3A4 and resid 405 and name CB) (segid 3A4 and resid 411 and name CA)	11.31	0.30	0.29
	assign (segid 3A4 and resid 405 and name CB) (segid 3A4 and resid 411 and name CB)	11.19	0.39	0.38
	assign (segid 3A4 and resid 405 and name CB) (segid 3A4 and resid 412 and name CA)	11.59	0.26	0.25
	assign (segid 3A4 and resid 405 and name CB) (segid 3A4 and resid 413 and name CA)	13.78	0.64	0.63
	assign (segid 3A4 and resid 405 and name CB) (segid 3A4 and resid 414 and name CA)	13.12	0.96	0.96
65	assign (segid 3A4 and resid 405 and name CB) (segid 3A4 and resid 415 and name CA)	15.42	0.94	0.93
	assign (segid 3A4 and resid 405 and name CB) (segid 3A4 and resid 415 and name CB)	16.49	0.73	0.73
	assign (segid 3A4 and resid 405 and name CB) (segid 3A4 and resid 434 and name CA)	16.99	0.86	0.86
	assign (segid 3A4 and resid 405 and name CB) (segid 3A4 and resid 435 and name CA)	16.54	0.68	0.68
	assign (segid 3A4 and resid 405 and name CB) (segid 3A4 and resid 437 and name CA)	18.51	0.62	0.63
70	assign (segid 3A4 and resid 405 and name CB) (segid 3A4 and resid 438 and name CA)	16.19	0.63	0.64
	assign (segid 3A4 and resid 405 and name CB) (segid 3A4 and resid 439 and name CA)	17.35	0.65	0.64
	assign (segid 3A4 and resid 405 and name CB) (segid 3A4 and resid 440 and name CA)	15.52	0.53	0.53
	assign (segid 3A4 and resid 405 and name N) (segid 3A4 and resid 405 and name C)	2.47	0.05	0.04
	assign (segid 3A4 and resid 405 and name N) (segid 3A4 and resid 405 and name CA)	1.46	0.01	0.00
75	assign (segid 3A4 and resid 405 and name N) (segid 3A4 and resid 405 and name CB)	2.45	0.01	0.02
	assign (segid 3A4 and resid 405 and name N) (segid 3A4 and resid 405 and name O)	3.49	0.08	0.09
	assign (segid 3A4 and resid 405 and name N) (segid 3A4 and resid 406 and name C)	4.74	0.07	0.06
	assign (segid 3A4 and resid 405 and name N) (segid 3A4 and resid 406 and name CA)	4.25	0.03	0.04
	assign (segid 3A4 and resid 405 and name N) (segid 3A4 and resid 406 and name N)	2.85	0.03	0.02
80	assign (segid 3A4 and resid 405 and name N) (segid 3A4 and resid 406 and name O)	5.82	0.12	0.12
	assign (segid 3A4 and resid 405 and name N) (segid 3A4 and resid 407 and name C)	5.62	0.04	0.05
	assign (segid 3A4 and resid 405 and name N) (segid 3A4 and resid 407 and name CA)	5.38	0.04	0.05
	assign (segid 3A4 and resid 405 and name N) (segid 3A4 and resid 407 and name CB)	5.62	0.11	0.11

	assign (segid 3A4 and resid 106 and name N)	(segid 3A4 and resid 406 and name CA)	1.46	0.01	0.01
	assign (segid 3A4 and resid 406 and name N)	(segid 3A4 and resid 406 and name O)	3.49	0.04	0.04
	assign (segid 3A4 and resid 406 and name N)	(segid 3A4 and resid 407 and name C)	4.78	0.04	0.04
	assign (segid 3A4 and resid 406 and name N)	(segid 3A4 and resid 407 and name CA)	4.21	0.07	0.07
5	assign (segid 3A4 and resid 406 and name N)	(segid 3A4 and resid 407 and name CB)	5.02	0.12	0.12
	assign (segid 3A4 and resid 406 and name N)	(segid 3A4 and resid 407 and name N)	2.81	0.08	0.09
	assign (segid 3A4 and resid 406 and name N)	(segid 3A4 and resid 407 and name O)	5.89	0.08	0.08
	assign (segid 3A4 and resid 406 and name N)	(segid 3A4 and resid 407 and name C)	5.92	0.23	0.22
	assign (segid 3A4 and resid 406 and name N)	(segid 3A4 and resid 408 and name C)	5.52	0.10	0.11
	assign (segid 3A4 and resid 406 and name N)	(segid 3A4 and resid 408 and name CA)	5.64	0.13	0.12
10	assign (segid 3A4 and resid 406 and name N)	(segid 3A4 and resid 408 and name CB)	4.45	0.07	0.06
	assign (segid 3A4 and resid 406 and name N)	(segid 3A4 and resid 408 and name N)	7.10	0.24	0.23
	assign (segid 3A4 and resid 406 and name N)	(segid 3A4 and resid 408 and name O)	6.76	0.36	0.36
	assign (segid 3A4 and resid 406 and name N)	(segid 3A4 and resid 409 and name C)	6.08	0.41	0.41
	assign (segid 3A4 and resid 406 and name N)	(segid 3A4 and resid 409 and name CA)	5.73	0.56	0.56
15	assign (segid 3A4 and resid 406 and name N)	(segid 3A4 and resid 409 and name CB)	5.80	0.61	0.61
	assign (segid 3A4 and resid 406 and name N)	(segid 3A4 and resid 409 and name CG)	5.22	0.32	0.32
	assign (segid 3A4 and resid 406 and name N)	(segid 3A4 and resid 409 and name N)	7.36	0.36	0.36
	assign (segid 3A4 and resid 406 and name N)	(segid 3A4 and resid 410 and name CA)	6.35	0.35	0.36
	assign (segid 3A4 and resid 406 and name N)	(segid 3A4 and resid 407 and name C)	3.23	0.26	0.26
20	assign (segid 3A4 and resid 406 and name O)	(segid 3A4 and resid 407 and name CA)	2.75	0.04	0.04
	assign (segid 3A4 and resid 406 and name O)	(segid 3A4 and resid 407 and name CB)	4.16	0.12	0.11
	assign (segid 3A4 and resid 406 and name O)	(segid 3A4 and resid 407 and name N)	2.24	0.01	0.01
	assign (segid 3A4 and resid 406 and name O)	(segid 3A4 and resid 407 and name O)	3.77	0.28	0.29
	assign (segid 3A4 and resid 406 and name O)	(segid 3A4 and resid 408 and name C)	4.68	0.60	0.61
25	assign (segid 3A4 and resid 406 and name O)	(segid 3A4 and resid 408 and name CA)	4.83	0.44	0.44
	assign (segid 3A4 and resid 406 and name O)	(segid 3A4 and resid 408 and name CB)	5.80	0.42	0.42
	assign (segid 3A4 and resid 406 and name O)	(segid 3A4 and resid 408 and name N)	3.77	0.34	0.34
	assign (segid 3A4 and resid 406 and name O)	(segid 3A4 and resid 408 and name O)	5.50	0.63	0.64
	assign (segid 3A4 and resid 406 and name O)	(segid 3A4 and resid 409 and name C)	4.55	0.78	0.78
30	assign (segid 3A4 and resid 406 and name O)	(segid 3A4 and resid 409 and name CA)	4.65	0.79	0.78
	assign (segid 3A4 and resid 406 and name O)	(segid 3A4 and resid 409 and name CB)	4.83	0.87	0.87
	assign (segid 3A4 and resid 406 and name O)	(segid 3A4 and resid 409 and name CG)	5.77	0.81	0.80
	assign (segid 3A4 and resid 406 and name O)	(segid 3A4 and resid 409 and name N)	4.07	0.68	0.68
	assign (segid 3A4 and resid 406 and name O)	(segid 3A4 and resid 409 and name O)	5.62	0.76	0.76
35	assign (segid 3A4 and resid 406 and name O)	(segid 3A4 and resid 410 and name C)	5.45	0.61	0.61
	assign (segid 3A4 and resid 406 and name O)	(segid 3A4 and resid 410 and name CA)	4.29	0.69	0.69
	assign (segid 3A4 and resid 406 and name O)	(segid 3A4 and resid 410 and name N)	3.67	0.76	0.77
	assign (segid 3A4 and resid 406 and name O)	(segid 3A4 and resid 410 and name O)	6.50	0.60	0.59
40	assign (segid 3A4 and resid 406 and name O)	(segid 3A4 and resid 411 and name CA)	6.84	0.55	0.54
	assign (segid 3A4 and resid 406 and name O)	(segid 3A4 and resid 411 and name CB)	6.98	0.47	0.47
	assign (segid 3A4 and resid 406 and name O)	(segid 3A4 and resid 411 and name N)	5.54	0.57	0.58
	assign (segid 3A4 and resid 406 and name O)	(segid 3A4 and resid 407 and name CB)	2.50	0.03	0.02
	assign (segid 3A4 and resid 407 and name C)	(segid 3A4 and resid 407 and name O)	1.24	0.01	0.02
45	assign (segid 3A4 and resid 407 and name C)	(segid 3A4 and resid 408 and name C)	3.05	0.09	0.09
	assign (segid 3A4 and resid 407 and name C)	(segid 3A4 and resid 408 and name CA)	2.44	0.02	0.02
	assign (segid 3A4 and resid 407 and name C)	(segid 3A4 and resid 408 and name CB)	3.73	0.02	0.02
	assign (segid 3A4 and resid 407 and name C)	(segid 3A4 and resid 408 and name N)	1.33	0.01	0.01
	assign (segid 3A4 and resid 407 and name C)	(segid 3A4 and resid 408 and name O)	3.77	0.12	0.11
50	assign (segid 3A4 and resid 407 and name C)	(segid 3A4 and resid 409 and name C)	4.81	0.24	0.24
	assign (segid 3A4 and resid 407 and name C)	(segid 3A4 and resid 409 and name CA)	4.65	0.18	0.18
	assign (segid 3A4 and resid 407 and name C)	(segid 3A4 and resid 409 and name CB)	5.55	0.18	0.19
	assign (segid 3A4 and resid 407 and name C)	(segid 3A4 and resid 409 and name CD2)	7.16	0.11	0.10
	assign (segid 3A4 and resid 407 and name C)	(segid 3A4 and resid 409 and name CG)	6.24	0.13	0.13
55	assign (segid 3A4 and resid 407 and name C)	(segid 3A4 and resid 409 and name N)	3.43	0.15	0.15
	assign (segid 3A4 and resid 407 and name C)	(segid 3A4 and resid 409 and name O)	5.95	0.19	0.20
	assign (segid 3A4 and resid 407 and name C)	(segid 3A4 and resid 410 and name C)	5.15	0.33	0.33
	assign (segid 3A4 and resid 407 and name C)	(segid 3A4 and resid 410 and name CA)	4.77	0.38	0.38
	assign (segid 3A4 and resid 407 and name C)	(segid 3A4 and resid 410 and name N)	4.01	0.36	0.36
60	assign (segid 3A4 and resid 407 and name C)	(segid 3A4 and resid 410 and name O)	6.32	0.32	0.32
	assign (segid 3A4 and resid 407 and name C)	(segid 3A4 and resid 411 and name C)	6.28	0.35	0.34
	assign (segid 3A4 and resid 407 and name C)	(segid 3A4 and resid 411 and name CA)	5.31	0.30	0.31
	assign (segid 3A4 and resid 407 and name C)	(segid 3A4 and resid 411 and name CB)	4.85	0.32	0.32
	assign (segid 3A4 and resid 407 and name C)	(segid 3A4 and resid 411 and name N)	4.47	0.31	0.31
65	assign (segid 3A4 and resid 407 and name C)	(segid 3A4 and resid 412 and name N)	6.15	0.45	0.44
	assign (segid 3A4 and resid 407 and name CA)	(segid 3A4 and resid 407 and name C)	1.51	0.01	0.02
	assign (segid 3A4 and resid 407 and name CA)	(segid 3A4 and resid 407 and name CB)	1.54	0.01	0.00
	assign (segid 3A4 and resid 407 and name CA)	(segid 3A4 and resid 407 and name O)	2.38	0.02	0.02
	assign (segid 3A4 and resid 407 and name CA)	(segid 3A4 and resid 408 and name C)	4.44	0.08	0.08
70	assign (segid 3A4 and resid 407 and name CA)	(segid 3A4 and resid 408 and name CA)	3.82	0.02	0.02
	assign (segid 3A4 and resid 407 and name CA)	(segid 3A4 and resid 408 and name CB)	4.91	0.06	0.05
	assign (segid 3A4 and resid 407 and name CA)	(segid 3A4 and resid 408 and name N)	2.45	0.02	0.02
	assign (segid 3A4 and resid 407 and name CA)	(segid 3A4 and resid 408 and name O)	5.22	0.12	0.11
	assign (segid 3A4 and resid 407 and name CA)	(segid 3A4 and resid 409 and name C)	5.73	0.32	0.32
75	assign (segid 3A4 and resid 407 and name CA)	(segid 3A4 and resid 409 and name CA)	5.67	0.22	0.22
	assign (segid 3A4 and resid 407 and name CA)	(segid 3A4 and resid 409 and name CB)	6.32	0.25	0.25
	assign (segid 3A4 and resid 407 and name CA)	(segid 3A4 and resid 409 and name CG)	7.03	0.17	0.17
	assign (segid 3A4 and resid 407 and name CA)	(segid 3A4 and resid 409 and name N)	4.55	0.15	0.15
	assign (segid 3A4 and resid 407 and name CA)	(segid 3A4 and resid 409 and name O)	6.88	0.31	0.31
80	assign (segid 3A4 and resid 407 and name CA)	(segid 3A4 and resid 410 and name C)	5.93	0.46	0.46
	assign (segid 3A4 and resid 407 and name CA)	(segid 3A4 and resid 410 and name CA)	5.33	0.52	0.53
	assign (segid 3A4 and resid 407 and name CA)	(segid 3A4 and resid 410 and name N)	4.77	0.44	0.45
	assign (segid 3A4 and resid 407 and name CA)	(segid 3A4 and resid 411 and name CA)	6.39	0.40	0.41

	assign (segid 3A4 and resid 407 and name CA)	(segid 3A4 and resid 411 and name CB)	5.94	0.40	0.40
	assign (segid 3A4 and resid 407 and name CA)	(segid 3A4 and resid 411 and name N)	5.49	0.41	0.41
	assign (segid 3A4 and resid 407 and name CA)	(segid 3A4 and resid 412 and name CA)	8.72	0.49	0.49
	assign (segid 3A4 and resid 407 and name CA)	(segid 3A4 and resid 413 and name CA)	12.88	1.02	1.02
	assign (segid 3A4 and resid 407 and name CA)	(segid 3A4 and resid 414 and name CA)	13.46	1.47	1.47
5	assign (segid 3A4 and resid 407 and name CA)	(segid 3A4 and resid 415 and name CA)	16.61	1.25	1.25
	assign (segid 3A4 and resid 407 and name CA)	(segid 3A4 and resid 415 and name CB)	17.55	1.21	1.20
	assign (segid 3A4 and resid 407 and name CA)	(segid 3A4 and resid 440 and name CA)	16.46	0.74	0.74
	assign (segid 3A4 and resid 407 and name CB)	(segid 3A4 and resid 408 and name C)	5.47	0.08	0.08
	assign (segid 3A4 and resid 407 and name CB)	(segid 3A4 and resid 408 and name CA)	4.53	0.08	0.08
10	assign (segid 3A4 and resid 407 and name CB)	(segid 3A4 and resid 408 and name CB)	5.48	0.14	0.13
	assign (segid 3A4 and resid 407 and name CB)	(segid 3A4 and resid 408 and name N)	3.23	0.08	0.09
	assign (segid 3A4 and resid 407 and name CB)	(segid 3A4 and resid 408 and name O)	6.18	0.13	0.13
	assign (segid 3A4 and resid 407 and name CB)	(segid 3A4 and resid 409 and name C)	7.13	0.29	0.29
	assign (segid 3A4 and resid 407 and name CB)	(segid 3A4 and resid 409 and name CB)	7.02	0.16	0.16
15	assign (segid 3A4 and resid 407 and name CB)	(segid 3A4 and resid 409 and name N)	7.73	0.19	0.20
	assign (segid 3A4 and resid 407 and name CB)	(segid 3A4 and resid 409 and name N)	5.80	0.11	0.11
	assign (segid 3A4 and resid 407 and name CB)	(segid 3A4 and resid 410 and name CA)	6.64	0.55	0.55
	assign (segid 3A4 and resid 407 and name CB)	(segid 3A4 and resid 410 and name N)	6.17	0.44	0.44
	assign (segid 3A4 and resid 407 and name CB)	(segid 3A4 and resid 410 and name N)	7.14	0.45	0.45
20	assign (segid 3A4 and resid 407 and name CB)	(segid 3A4 and resid 411 and name CB)	6.40	0.46	0.46
	assign (segid 3A4 and resid 407 and name CB)	(segid 3A4 and resid 411 and name N)	6.46	0.45	0.45
	assign (segid 3A4 and resid 407 and name CB)	(segid 3A4 and resid 412 and name CA)	9.61	0.50	0.51
	assign (segid 3A4 and resid 407 and name CB)	(segid 3A4 and resid 413 and name CA)	13.94	0.97	0.96
	assign (segid 3A4 and resid 407 and name CB)	(segid 3A4 and resid 414 and name CA)	14.36	1.43	1.43
25	assign (segid 3A4 and resid 407 and name CB)	(segid 3A4 and resid 415 and name CA)	17.44	1.17	1.17
	assign (segid 3A4 and resid 407 and name CB)	(segid 3A4 and resid 440 and name CA)	16.87	0.72	0.73
	assign (segid 3A4 and resid 407 and name CB)	(segid 3A4 and resid 407 and name C)	2.49	0.02	0.02
	assign (segid 3A4 and resid 407 and name N)	(segid 3A4 and resid 407 and name CA)	1.45	0.00	0.01
	assign (segid 3A4 and resid 407 and name N)	(segid 3A4 and resid 407 and name CB)	2.46	0.02	0.02
30	assign (segid 3A4 and resid 407 and name N)	(segid 3A4 and resid 407 and name O)	3.54	0.03	0.04
	assign (segid 3A4 and resid 407 and name N)	(segid 3A4 and resid 408 and name C)	1.83	0.08	0.08
	assign (segid 3A4 and resid 407 and name N)	(segid 3A4 and resid 408 and name CA)	4.28	0.01	0.02
	assign (segid 3A4 and resid 407 and name N)	(segid 3A4 and resid 408 and name CB)	5.06	0.07	0.07
	assign (segid 3A4 and resid 407 and name N)	(segid 3A4 and resid 408 and name N)	2.87	0.02	0.01
35	assign (segid 3A4 and resid 407 and name N)	(segid 3A4 and resid 408 and name O)	5.82	0.12	0.11
	assign (segid 3A4 and resid 407 and name N)	(segid 3A4 and resid 409 and name C)	5.92	0.30	0.30
	assign (segid 3A4 and resid 407 and name N)	(segid 3A4 and resid 409 and name CA)	5.67	0.22	0.21
	assign (segid 3A4 and resid 407 and name N)	(segid 3A4 and resid 409 and name CB)	5.98	0.30	0.29
	assign (segid 3A4 and resid 407 and name N)	(segid 3A4 and resid 409 and name CG)	6.54	0.24	0.25
40	assign (segid 3A4 and resid 407 and name N)	(segid 3A4 and resid 409 and name N)	4.59	0.14	0.15
	assign (segid 3A4 and resid 407 and name N)	(segid 3A4 and resid 409 and name O)	7.09	0.31	0.30
	assign (segid 3A4 and resid 407 and name N)	(segid 3A4 and resid 410 and name C)	6.69	0.11	0.41
	assign (segid 3A4 and resid 407 and name N)	(segid 3A4 and resid 410 and name CA)	5.82	0.48	0.48
	assign (segid 3A4 and resid 407 and name N)	(segid 3A4 and resid 410 and name N)	5.09	0.40	0.40
45	assign (segid 3A4 and resid 407 and name N)	(segid 3A4 and resid 411 and name CB)	7.17	0.34	0.34
	assign (segid 3A4 and resid 407 and name N)	(segid 3A4 and resid 411 and name N)	6.40	0.34	0.34
	assign (segid 3A4 and resid 407 and name O)	(segid 3A4 and resid 407 and name CB)	3.22	0.06	0.05
	assign (segid 3A4 and resid 407 and name O)	(segid 3A4 and resid 408 and name C)	3.00	0.17	0.17
	assign (segid 3A4 and resid 407 and name O)	(segid 3A4 and resid 408 and name CA)	2.77	0.05	0.04
50	assign (segid 3A4 and resid 407 and name O)	(segid 3A4 and resid 408 and name CB)	4.25	0.02	0.02
	assign (segid 3A4 and resid 407 and name O)	(segid 3A4 and resid 408 and name N)	2.25	0.02	0.02
	assign (segid 3A4 and resid 407 and name O)	(segid 3A4 and resid 408 and name O)	3.32	0.19	0.19
	assign (segid 3A4 and resid 407 and name O)	(segid 3A4 and resid 409 and name C)	4.46	0.34	0.34
	assign (segid 3A4 and resid 407 and name O)	(segid 3A4 and resid 409 and name CA)	4.60	0.30	0.30
55	assign (segid 3A4 and resid 407 and name O)	(segid 3A4 and resid 409 and name CB)	5.73	0.26	0.27
	assign (segid 3A4 and resid 407 and name O)	(segid 3A4 and resid 409 and name CD2)	7.38	0.18	0.17
	assign (segid 3A4 and resid 407 and name O)	(segid 3A4 and resid 409 and name CG)	6.59	0.25	0.25
	assign (segid 3A4 and resid 407 and name O)	(segid 3A4 and resid 409 and name N)	3.60	0.24	0.23
	assign (segid 3A4 and resid 407 and name O)	(segid 3A4 and resid 409 and name O)	5.49	0.29	0.29
60	assign (segid 3A4 and resid 407 and name O)	(segid 3A4 and resid 410 and name C)	4.20	0.40	0.41
	assign (segid 3A4 and resid 407 and name O)	(segid 3A4 and resid 410 and name CA)	4.11	0.43	0.43
	assign (segid 3A4 and resid 407 and name O)	(segid 3A4 and resid 410 and name N)	3.58	0.43	0.43
	assign (segid 3A4 and resid 407 and name O)	(segid 3A4 and resid 410 and name O)	5.33	0.38	0.38
	assign (segid 3A4 and resid 407 and name O)	(segid 3A4 and resid 411 and name C)	5.22	0.44	0.44
65	assign (segid 3A4 and resid 407 and name O)	(segid 3A4 and resid 411 and name CA)	4.17	0.38	0.37
	assign (segid 3A4 and resid 407 and name O)	(segid 3A4 and resid 411 and name CB)	3.71	0.34	0.34
	assign (segid 3A4 and resid 407 and name O)	(segid 3A4 and resid 411 and name N)	3.42	0.41	0.40
	assign (segid 3A4 and resid 407 and name O)	(segid 3A4 and resid 411 and name O)	6.29	0.40	0.40
	assign (segid 3A4 and resid 407 and name O)	(segid 3A4 and resid 412 and name N)	5.25	0.54	0.54
70	assign (segid 3A4 and resid 408 and name C)	(segid 3A4 and resid 408 and name CB)	2.48	0.03	0.04
	assign (segid 3A4 and resid 408 and name C)	(segid 3A4 and resid 408 and name O)	1.24	0.02	0.01
	assign (segid 3A4 and resid 408 and name C)	(segid 3A4 and resid 409 and name C)	3.15	0.07	0.06
	assign (segid 3A4 and resid 408 and name C)	(segid 3A4 and resid 409 and name CA)	2.44	0.01	0.01
	assign (segid 3A4 and resid 408 and name C)	(segid 3A4 and resid 409 and name CB)	3.70	0.03	0.03
75	assign (segid 3A4 and resid 408 and name C)	(segid 3A4 and resid 409 and name CD2)	4.66	0.13	0.12
	assign (segid 3A4 and resid 408 and name C)	(segid 3A4 and resid 409 and name CG)	4.19	0.13	0.13
	assign (segid 3A4 and resid 408 and name C)	(segid 3A4 and resid 409 and name N)	1.32	0.02	0.02
	assign (segid 3A4 and resid 408 and name C)	(segid 3A4 and resid 409 and name O)	4.14	0.15	0.15
	assign (segid 3A4 and resid 408 and name C)	(segid 3A4 and resid 410 and name C)	4.65	0.06	0.06
80	assign (segid 3A4 and resid 408 and name C)	(segid 3A4 and resid 410 and name CA)	4.48	0.07	0.07
	assign (segid 3A4 and resid 408 and name C)	(segid 3A4 and resid 410 and name N)	3.24	0.07	0.08
	assign (segid 3A4 and resid 408 and name C)	(segid 3A4 and resid 410 and name O)	5.81	0.07	0.07

	assign (segid 3A4 and resid 408 and name C)	(segid 3A4 and resid 411 and name C)	4.89	0.13	0.13
	assign (segid 3A4 and resid 408 and name C)	(segid 3A4 and resid 411 and name CA)	4.64	0.06	0.06
	assign (segid 3A4 and resid 408 and name C)	(segid 3A4 and resid 411 and name CB)	4.63	0.26	0.26
	assign (segid 3A4 and resid 408 and name C)	(segid 3A4 and resid 411 and name N)	3.86	0.05	0.05
5	assign (segid 3A4 and resid 408 and name C)	(segid 3A4 and resid 411 and name O)	6.04	0.13	0.13
	assign (segid 3A4 and resid 408 and name C)	(segid 3A4 and resid 412 and name C)	5.31	0.61	0.62
	assign (segid 3A4 and resid 408 and name C)	(segid 3A4 and resid 412 and name CA)	4.98	0.34	0.34
	assign (segid 3A4 and resid 408 and name C)	(segid 3A4 and resid 412 and name N)	4.18	0.26	0.27
	assign (segid 3A4 and resid 408 and name C)	(segid 3A4 and resid 412 and name O)	5.04	0.69	0.70
10	assign (segid 3A4 and resid 408 and name C)	(segid 3A4 and resid 408 and name O)	1.53	0.01	0.01
	assign (segid 3A4 and resid 408 and name CA)	(segid 3A4 and resid 408 and name CB)	1.53	0.02	0.02
	assign (segid 3A4 and resid 408 and name CA)	(segid 3A4 and resid 408 and name O)	2.40	0.02	0.01
	assign (segid 3A4 and resid 408 and name CA)	(segid 3A4 and resid 409 and name C)	4.56	0.04	0.04
	assign (segid 3A4 and resid 408 and name CA)	(segid 3A4 and resid 409 and name CA)	3.82	0.00	0.01
	assign (segid 3A4 and resid 408 and name CA)	(segid 3A4 and resid 409 and name CB)	4.86	0.04	0.05
15	assign (segid 3A4 and resid 408 and name CA)	(segid 3A4 and resid 409 and name CD2)	5.68	0.17	0.17
	assign (segid 3A4 and resid 408 and name CA)	(segid 3A4 and resid 409 and name CG)	5.12	0.14	0.15
	assign (segid 3A4 and resid 408 and name CA)	(segid 3A4 and resid 409 and name N)	2.45	0.03	0.02
	assign (segid 3A4 and resid 408 and name CA)	(segid 3A4 and resid 409 and name O)	5.61	0.13	0.13
20	assign (segid 3A4 and resid 408 and name CA)	(segid 3A4 and resid 410 and name C)	5.70	0.07	0.06
	assign (segid 3A4 and resid 408 and name CA)	(segid 3A4 and resid 410 and name CA)	5.54	0.10	0.10
	assign (segid 3A4 and resid 408 and name CA)	(segid 3A4 and resid 410 and name N)	4.40	0.11	0.12
	assign (segid 3A4 and resid 408 and name CA)	(segid 3A4 and resid 410 and name O)	6.88	0.06	0.06
	assign (segid 3A4 and resid 408 and name CA)	(segid 3A4 and resid 411 and name C)	5.79	0.13	0.14
25	assign (segid 3A4 and resid 408 and name CA)	(segid 3A4 and resid 411 and name CA)	5.39	0.06	0.06
	assign (segid 3A4 and resid 408 and name CA)	(segid 3A4 and resid 411 and name CB)	4.95	0.23	0.24
	assign (segid 3A4 and resid 408 and name CA)	(segid 3A4 and resid 411 and name N)	4.77	0.05	0.06
	assign (segid 3A4 and resid 408 and name CA)	(segid 3A4 and resid 411 and name O)	6.88	0.15	0.15
	assign (segid 3A4 and resid 408 and name CA)	(segid 3A4 and resid 412 and name CA)	6.07	0.37	0.37
30	assign (segid 3A4 and resid 408 and name CA)	(segid 3A4 and resid 412 and name N)	5.27	0.28	0.28
	assign (segid 3A4 and resid 408 and name CA)	(segid 3A4 and resid 413 and name CA)	9.88	0.86	0.86
	assign (segid 3A4 and resid 408 and name CA)	(segid 3A4 and resid 414 and name CA)	9.94	1.35	1.34
	assign (segid 3A4 and resid 408 and name CA)	(segid 3A4 and resid 415 and name CA)	12.99	1.18	1.17
	assign (segid 3A4 and resid 408 and name CA)	(segid 3A4 and resid 415 and name CB)	13.97	1.10	1.11
35	assign (segid 3A4 and resid 408 and name CA)	(segid 3A4 and resid 416 and name CA)	15.10	1.24	1.24
	assign (segid 3A4 and resid 408 and name CA)	(segid 3A4 and resid 435 and name CA)	18.37	0.67	0.66
	assign (segid 3A4 and resid 408 and name CA)	(segid 3A4 and resid 437 and name CA)	18.22	0.86	0.85
	assign (segid 3A4 and resid 408 and name CA)	(segid 3A4 and resid 438 and name CA)	15.52	0.90	0.89
	assign (segid 3A4 and resid 408 and name CA)	(segid 3A4 and resid 439 and name CA)	15.28	0.75	0.74
40	assign (segid 3A4 and resid 408 and name CA)	(segid 3A4 and resid 440 and name CA)	12.68	0.75	0.75
	assign (segid 3A4 and resid 408 and name CB)	(segid 3A4 and resid 409 and name C)	5.46	0.07	0.08
	assign (segid 3A4 and resid 408 and name CB)	(segid 3A4 and resid 409 and name CA)	4.38	0.07	0.07
	assign (segid 3A4 and resid 408 and name CB)	(segid 3A4 and resid 409 and name CB)	5.15	0.11	0.11
	assign (segid 3A4 and resid 408 and name CB)	(segid 3A4 and resid 409 and name CD2)	5.35	0.24	0.25
45	assign (segid 3A4 and resid 408 and name CB)	(segid 3A4 and resid 409 and name CG)	4.96	0.21	0.22
	assign (segid 3A4 and resid 408 and name CB)	(segid 3A4 and resid 409 and name N)	3.08	0.07	0.08
	assign (segid 3A4 and resid 408 and name CB)	(segid 3A4 and resid 409 and name O)	6.45	0.18	0.18
	assign (segid 3A4 and resid 408 and name CB)	(segid 3A4 and resid 410 and name C)	7.04	0.07	0.07
	assign (segid 3A4 and resid 408 and name CB)	(segid 3A4 and resid 410 and name CA)	6.83	0.08	0.07
50	assign (segid 3A4 and resid 408 and name CB)	(segid 3A4 and resid 410 and name N)	5.56	0.09	0.09
	assign (segid 3A4 and resid 408 and name CB)	(segid 3A4 and resid 411 and name C)	6.88	0.16	0.15
	assign (segid 3A4 and resid 408 and name CB)	(segid 3A4 and resid 411 and name CA)	6.69	0.12	0.12
	assign (segid 3A4 and resid 408 and name CB)	(segid 3A4 and resid 411 and name CB)	6.25	0.28	0.29
	assign (segid 3A4 and resid 408 and name CB)	(segid 3A4 and resid 411 and name N)	6.14	0.10	0.09
55	assign (segid 3A4 and resid 408 and name CB)	(segid 3A4 and resid 412 and name CA)	6.70	0.36	0.37
	assign (segid 3A4 and resid 408 and name CB)	(segid 3A4 and resid 412 and name N)	6.18	0.24	0.24
	assign (segid 3A4 and resid 408 and name CB)	(segid 3A4 and resid 413 and name CA)	9.93	0.82	0.83
	assign (segid 3A4 and resid 408 and name CB)	(segid 3A4 and resid 414 and name CA)	9.49	1.16	1.15
	assign (segid 3A4 and resid 408 and name CB)	(segid 3A4 and resid 415 and name CA)	12.28	1.03	1.04
60	assign (segid 3A4 and resid 408 and name CB)	(segid 3A4 and resid 415 and name CB)	13.34	0.94	0.93
	assign (segid 3A4 and resid 408 and name CB)	(segid 3A4 and resid 416 and name CA)	14.16	1.20	1.21
	assign (segid 3A4 and resid 408 and name CB)	(segid 3A4 and resid 417 and name CA)	17.02	1.37	1.38
	assign (segid 3A4 and resid 408 and name CB)	(segid 3A4 and resid 434 and name CA)	18.32	0.88	0.87
	assign (segid 3A4 and resid 408 and name CB)	(segid 3A4 and resid 435 and name CA)	16.88	0.66	0.65
65	assign (segid 3A4 and resid 408 and name CB)	(segid 3A4 and resid 436 and name CA)	18.29	0.83	0.83
	assign (segid 3A4 and resid 408 and name CB)	(segid 3A4 and resid 437 and name CA)	16.86	0.78	0.79
	assign (segid 3A4 and resid 408 and name CB)	(segid 3A4 and resid 438 and name CA)	14.19	0.83	0.84
	assign (segid 3A4 and resid 408 and name CB)	(segid 3A4 and resid 439 and name CA)	14.17	0.67	0.66
	assign (segid 3A4 and resid 408 and name CB)	(segid 3A4 and resid 440 and name CA)	11.76	0.65	0.65
70	assign (segid 3A4 and resid 408 and name N)	(segid 3A4 and resid 408 and name C)	2.46	0.03	0.04
	assign (segid 3A4 and resid 408 and name N)	(segid 3A4 and resid 408 and name CA)	1.46	0.01	0.00
	assign (segid 3A4 and resid 408 and name N)	(segid 3A4 and resid 408 and name CB)	2.48	0.03	0.03
	assign (segid 3A4 and resid 408 and name N)	(segid 3A4 and resid 408 and name O)	3.44	0.04	0.05
	assign (segid 3A4 and resid 408 and name N)	(segid 3A4 and resid 409 and name C)	4.87	0.12	0.12
75	assign (segid 3A4 and resid 408 and name N)	(segid 3A4 and resid 409 and name CA)	4.30	0.09	0.09
	assign (segid 3A4 and resid 408 and name N)	(segid 3A4 and resid 409 and name CB)	5.13	0.13	0.13
	assign (segid 3A4 and resid 408 and name N)	(segid 3A4 and resid 409 and name CD2)	6.37	0.16	0.16
	assign (segid 3A4 and resid 408 and name N)	(segid 3A4 and resid 409 and name CG)	5.52	0.08	0.09
	assign (segid 3A4 and resid 408 and name N)	(segid 3A4 and resid 409 and name N)	2.89	0.09	0.08
80	assign (segid 3A4 and resid 408 and name N)	(segid 3A4 and resid 409 and name O)	6.03	0.08	0.08
	assign (segid 3A4 and resid 408 and name N)	(segid 3A4 and resid 410 and name C)	5.93	0.16	0.16
	assign (segid 3A4 and resid 408 and name N)	(segid 3A4 and resid 410 and name CA)	5.43	0.23	0.23
	assign (segid 3A4 and resid 408 and name N)	(segid 3A4 and resid 410 and name N)	4.40	0.23	0.22

	assign (segid 3A4 and resid 408 and name N)	(segid 3A4 and resid 410 and name O)	7.04	0.15	0.16
	assign (segid 3A4 and resid 408 and name N)	(segid 3A4 and resid 411 and name C)	6.57	0.20	0.21
	assign (segid 3A4 and resid 408 and name N)	(segid 3A4 and resid 411 and name CA)	5.86	0.14	0.15
	assign (segid 3A4 and resid 408 and name N)	(segid 3A4 and resid 411 and name CB)	5.40	0.24	0.24
5	assign (segid 3A4 and resid 408 and name N)	(segid 3A4 and resid 411 and name N)	5.07	0.14	0.14
	assign (segid 3A4 and resid 408 and name N)	(segid 3A4 and resid 412 and name N)	6.22	0.34	0.33
	assign (segid 3A4 and resid 408 and name N)	(segid 3A4 and resid 408 and name CB)	3.34	0.05	0.05
	assign (segid 3A4 and resid 408 and name O)	(segid 3A4 and resid 409 and name C)	3.10	0.13	0.14
	assign (segid 3A4 and resid 408 and name O)	(segid 3A4 and resid 409 and name CA)	2.77	0.03	0.04
10	assign (segid 3A4 and resid 408 and name O)	(segid 3A4 and resid 409 and name CB)	4.24	0.05	0.04
	assign (segid 3A4 and resid 408 and name O)	(segid 3A4 and resid 409 and name CD2)	5.04	0.13	0.13
	assign (segid 3A4 and resid 408 and name O)	(segid 3A4 and resid 409 and name CG)	4.84	0.16	0.16
	assign (segid 3A4 and resid 408 and name O)	(segid 3A4 and resid 409 and name N)	2.24	0.01	0.01
	assign (segid 3A4 and resid 408 and name O)	(segid 3A4 and resid 409 and name O)	3.84	0.26	0.26
15	assign (segid 3A4 and resid 408 and name O)	(segid 3A4 and resid 410 and name C)	4.10	0.16	0.16
	assign (segid 3A4 and resid 408 and name O)	(segid 3A4 and resid 410 and name CA)	4.31	0.15	0.15
	assign (segid 3A4 and resid 408 and name O)	(segid 3A4 and resid 410 and name N)	3.30	0.08	0.08
	assign (segid 3A4 and resid 408 and name O)	(segid 3A4 and resid 410 and name O)	5.15	0.14	0.14
	assign (segid 3A4 and resid 408 and name O)	(segid 3A4 and resid 411 and name C)	3.74	0.11	0.11
20	assign (segid 3A4 and resid 408 and name O)	(segid 3A4 and resid 411 and name CA)	3.70	0.12	0.12
	assign (segid 3A4 and resid 408 and name O)	(segid 3A4 and resid 411 and name CB)	3.81	0.31	0.30
	assign (segid 3A4 and resid 408 and name O)	(segid 3A4 and resid 411 and name N)	3.16	0.16	0.16
	assign (segid 3A4 and resid 408 and name O)	(segid 3A4 and resid 411 and name O)	4.87	0.12	0.12
	assign (segid 3A4 and resid 408 and name O)	(segid 3A4 and resid 412 and name C)	4.33	0.61	0.60
25	assign (segid 3A4 and resid 408 and name O)	(segid 3A4 and resid 412 and name CA)	3.81	0.37	0.37
	assign (segid 3A4 and resid 408 and name O)	(segid 3A4 and resid 412 and name N)	2.99	0.27	0.28
	assign (segid 3A4 and resid 408 and name O)	(segid 3A4 and resid 412 and name O)	4.19	0.66	0.66
	assign (segid 3A4 and resid 409 and name C)	(segid 3A4 and resid 409 and name CB)	2.50	0.04	0.04
	assign (segid 3A4 and resid 409 and name C)	(segid 3A4 and resid 409 and name CD2)	4.40	0.08	0.08
30	assign (segid 3A4 and resid 409 and name C)	(segid 3A4 and resid 409 and name CG)	3.87	0.05	0.04
	assign (segid 3A4 and resid 409 and name C)	(segid 3A4 and resid 409 and name O)	1.23	0.00	0.01
	assign (segid 3A4 and resid 409 and name C)	(segid 3A4 and resid 410 and name C)	3.09	0.03	0.04
	assign (segid 3A4 and resid 409 and name C)	(segid 3A4 and resid 410 and name CA)	2.42	0.01	0.01
35	assign (segid 3A4 and resid 409 and name C)	(segid 3A4 and resid 410 and name N)	1.33	0.01	0.01
	assign (segid 3A4 and resid 409 and name C)	(segid 3A4 and resid 410 and name O)	4.03	0.09	0.09
	assign (segid 3A4 and resid 409 and name C)	(segid 3A4 and resid 411 and name C)	4.76	0.11	0.11
	assign (segid 3A4 and resid 409 and name C)	(segid 3A4 and resid 411 and name CA)	4.53	0.07	0.07
	assign (segid 3A4 and resid 409 and name C)	(segid 3A4 and resid 411 and name CB)	5.41	0.18	0.18
40	assign (segid 3A4 and resid 409 and name C)	(segid 3A4 and resid 411 and name N)	3.28	0.07	0.07
	assign (segid 3A4 and resid 409 and name C)	(segid 3A4 and resid 411 and name O)	5.91	0.13	0.13
	assign (segid 3A4 and resid 409 and name C)	(segid 3A4 and resid 412 and name C)	4.70	0.35	0.34
	assign (segid 3A4 and resid 409 and name C)	(segid 3A4 and resid 412 and name CA)	4.93	0.16	0.16
	assign (segid 3A4 and resid 409 and name C)	(segid 3A4 and resid 412 and name N)	4.07	0.14	0.13
	assign (segid 3A4 and resid 409 and name C)	(segid 3A4 and resid 412 and name O)	4.32	0.25	0.25
45	assign (segid 3A4 and resid 409 and name C)	(segid 3A4 and resid 409 and name C)	1.51	0.01	0.02
	assign (segid 3A4 and resid 409 and name CA)	(segid 3A4 and resid 409 and name CB)	1.53	0.02	0.02
	assign (segid 3A4 and resid 409 and name CA)	(segid 3A4 and resid 409 and name CD2)	3.14	0.08	0.09
	assign (segid 3A4 and resid 409 and name CA)	(segid 3A4 and resid 409 and name CG)	2.57	0.04	0.04
	assign (segid 3A4 and resid 409 and name CA)	(segid 3A4 and resid 409 and name O)	2.38	0.02	0.02
50	assign (segid 3A4 and resid 409 and name CA)	(segid 3A4 and resid 410 and name C)	4.41	0.03	0.03
	assign (segid 3A4 and resid 409 and name CA)	(segid 3A4 and resid 410 and name CA)	3.79	0.03	0.02
	assign (segid 3A4 and resid 409 and name CA)	(segid 3A4 and resid 410 and name N)	2.42	0.03	0.04
	assign (segid 3A4 and resid 409 and name CA)	(segid 3A4 and resid 410 and name O)	5.43	0.09	0.09
	assign (segid 3A4 and resid 409 and name CA)	(segid 3A4 and resid 411 and name C)	5.47	0.15	0.15
55	assign (segid 3A4 and resid 409 and name CA)	(segid 3A4 and resid 411 and name CA)	5.38	0.09	0.10
	assign (segid 3A4 and resid 409 and name CA)	(segid 3A4 and resid 411 and name CB)	6.00	0.25	0.24
	assign (segid 3A4 and resid 409 and name CA)	(segid 3A4 and resid 411 and name N)	4.27	0.08	0.08
	assign (segid 3A4 and resid 409 and name CA)	(segid 3A4 and resid 411 and name O)	6.63	0.18	0.18
	assign (segid 3A4 and resid 409 and name CA)	(segid 3A4 and resid 412 and name C)	4.92	0.54	0.54
60	assign (segid 3A4 and resid 409 and name CA)	(segid 3A4 and resid 412 and name CA)	5.19	0.25	0.26
	assign (segid 3A4 and resid 409 and name CA)	(segid 3A4 and resid 412 and name N)	4.56	0.19	0.19
	assign (segid 3A4 and resid 409 and name CA)	(segid 3A4 and resid 412 and name O)	4.36	0.53	0.53
	assign (segid 3A4 and resid 409 and name CA)	(segid 3A4 and resid 413 and name CA)	7.97	0.92	0.92
65	assign (segid 3A4 and resid 409 and name CA)	(segid 3A4 and resid 414 and name CA)	8.77	1.59	1.58
	assign (segid 3A4 and resid 409 and name CA)	(segid 3A4 and resid 415 and name CA)	12.02	1.52	1.53
	assign (segid 3A4 and resid 409 and name CA)	(segid 3A4 and resid 415 and name CB)	12.90	1.51	1.50
	assign (segid 3A4 and resid 409 and name CA)	(segid 3A4 and resid 416 and name CA)	14.65	1.49	1.48
	assign (segid 3A4 and resid 409 and name CA)	(segid 3A4 and resid 438 and name CA)	16.65	0.72	0.72
	assign (segid 3A4 and resid 409 and name CA)	(segid 3A4 and resid 439 and name CA)	16.29	0.68	0.68
70	assign (segid 3A4 and resid 409 and name CA)	(segid 3A4 and resid 440 and name CA)	13.24	0.72	0.72
	assign (segid 3A4 and resid 409 and name CB)	(segid 3A4 and resid 409 and name CD2)	2.52	0.03	0.03
	assign (segid 3A4 and resid 409 and name CB)	(segid 3A4 and resid 409 and name CG)	1.52	0.02	0.02
	assign (segid 3A4 and resid 409 and name CB)	(segid 3A4 and resid 410 and name C)	5.55	0.06	0.07
	assign (segid 3A4 and resid 409 and name CB)	(segid 3A4 and resid 410 and name CA)	4.63	0.09	0.09
75	assign (segid 3A4 and resid 409 and name CB)	(segid 3A4 and resid 410 and name N)	3.35	0.10	0.10
	assign (segid 3A4 and resid 409 and name CB)	(segid 3A4 and resid 410 and name O)	6.49	0.10	0.10
	assign (segid 3A4 and resid 409 and name CB)	(segid 3A4 and resid 411 and name C)	6.91	0.15	0.15
	assign (segid 3A4 and resid 409 and name CB)	(segid 3A4 and resid 411 and name CA)	6.82	0.07	0.08
	assign (segid 3A4 and resid 409 and name CB)	(segid 3A4 and resid 411 and name CB)	7.48	0.22	0.21
80	assign (segid 3A4 and resid 409 and name CB)	(segid 3A4 and resid 411 and name N)	5.63	0.08	0.08
	assign (segid 3A4 and resid 409 and name CB)	(segid 3A4 and resid 412 and name C)	5.98	0.58	0.58
	assign (segid 3A4 and resid 409 and name CB)	(segid 3A4 and resid 412 and name CA)	6.48	0.30	0.30
	assign (segid 3A4 and resid 409 and name CB)	(segid 3A4 and resid 412 and name N)	5.98	0.21	0.20

	assign (segid 3A4 and resid 409 and name CB)	(segid 3A4 and resid 112 and name O)	5.25	0.56	0.55
	assign (segid 3A4 and resid 109 and name CB)	(segid 3A4 and resid 113 and name CA)	8.53	0.89	0.90
	assign (segid 3A4 and resid 109 and name CB)	(segid 3A4 and resid 414 and name CA)	9.21	1.59	1.59
	assign (segid 3A4 and resid 409 and name CB)	(segid 3A4 and resid 415 and name CA)	12.26	1.66	1.66
5	assign (segid 3A4 and resid 409 and name CB)	(segid 3A4 and resid 415 and name CB)	13.14	1.63	1.64
	assign (segid 3A4 and resid 409 and name CB)	(segid 3A4 and resid 416 and name CA)	14.84	1.68	1.68
	assign (segid 3A4 and resid 409 and name CB)	(segid 3A4 and resid 438 and name CA)	16.86	0.76	0.77
	assign (segid 3A4 and resid 409 and name CB)	(segid 3A4 and resid 439 and name CA)	16.75	0.78	0.77
	assign (segid 3A4 and resid 409 and name CB)	(segid 3A4 and resid 440 and name CA)	13.79	0.83	0.82
10	assign (segid 3A4 and resid 409 and name CB)	(segid 3A4 and resid 410 and name C)	7.38	0.10	0.10
	assign (segid 3A4 and resid 409 and name CD2)	(segid 3A4 and resid 410 and name CA)	6.79	0.09	0.09
	assign (segid 3A4 and resid 409 and name CD2)	(segid 3A4 and resid 410 and name N)	5.50	0.10	0.10
	assign (segid 3A4 and resid 409 and name CD2)	(segid 3A4 and resid 411 and name N)	7.22	0.09	0.09
	assign (segid 3A4 and resid 409 and name CD2)	(segid 3A4 and resid 412 and name C)	5.96	0.73	0.73
15	assign (segid 3A4 and resid 409 and name CD2)	(segid 3A4 and resid 412 and name CA)	6.64	0.39	0.38
	assign (segid 3A4 and resid 409 and name CD2)	(segid 3A4 and resid 412 and name N)	6.64	0.26	0.26
	assign (segid 3A4 and resid 409 and name CD2)	(segid 3A4 and resid 412 and name O)	5.05	0.88	0.89
	assign (segid 3A4 and resid 409 and name CD2)	(segid 3A4 and resid 409 and name CD2)	1.48	0.05	0.05
	assign (segid 3A4 and resid 409 and name CG)	(segid 3A4 and resid 410 and name C)	6.92	0.06	0.05
20	assign (segid 3A4 and resid 409 and name CG)	(segid 3A4 and resid 410 and name CA)	6.09	0.09	0.09
	assign (segid 3A4 and resid 409 and name CG)	(segid 3A4 and resid 410 and name N)	4.74	0.09	0.10
	assign (segid 3A4 and resid 409 and name CG)	(segid 3A4 and resid 411 and name N)	6.83	0.12	0.12
	assign (segid 3A4 and resid 409 and name CG)	(segid 3A4 and resid 412 and name CA)	7.10	0.40	0.39
	assign (segid 3A4 and resid 409 and name CG)	(segid 3A4 and resid 412 and name N)	6.81	0.29	0.28
25	assign (segid 3A4 and resid 409 and name CG)	(segid 3A4 and resid 412 and name O)	5.71	0.78	0.78
	assign (segid 3A4 and resid 409 and name N)	(segid 3A4 and resid 409 and name C)	2.50	0.03	0.03
	assign (segid 3A4 and resid 409 and name N)	(segid 3A4 and resid 409 and name CA)	1.46	0.00	0.00
	assign (segid 3A4 and resid 409 and name N)	(segid 3A4 and resid 409 and name CB)	2.47	0.02	0.01
	assign (segid 3A4 and resid 409 and name N)	(segid 3A4 and resid 409 and name CD2)	3.81	0.12	0.12
30	assign (segid 3A4 and resid 409 and name N)	(segid 3A4 and resid 409 and name CG)	3.08	0.09	0.09
	assign (segid 3A4 and resid 409 and name N)	(segid 3A4 and resid 409 and name O)	3.59	0.05	0.04
	assign (segid 3A4 and resid 409 and name N)	(segid 3A4 and resid 410 and name C)	4.75	0.07	0.07
	assign (segid 3A4 and resid 409 and name N)	(segid 3A4 and resid 410 and name CA)	4.19	0.09	0.09
	assign (segid 3A4 and resid 409 and name N)	(segid 3A4 and resid 410 and name N)	2.77	0.09	0.10
35	assign (segid 3A4 and resid 409 and name N)	(segid 3A4 and resid 410 and name O)	5.91	0.10	0.09
	assign (segid 3A4 and resid 409 and name N)	(segid 3A4 and resid 411 and name C)	5.62	0.12	0.13
	assign (segid 3A4 and resid 409 and name N)	(segid 3A4 and resid 411 and name CA)	5.35	0.07	0.06
	assign (segid 3A4 and resid 409 and name N)	(segid 3A4 and resid 411 and name CB)	5.59	0.21	0.22
	assign (segid 3A4 and resid 409 and name N)	(segid 3A4 and resid 411 and name N)	4.30	0.07	0.08
40	assign (segid 3A4 and resid 409 and name N)	(segid 3A4 and resid 411 and name O)	6.82	0.13	0.12
	assign (segid 3A4 and resid 409 and name N)	(segid 3A4 and resid 412 and name C)	5.64	0.59	0.60
	assign (segid 3A4 and resid 409 and name N)	(segid 3A4 and resid 412 and name CA)	5.59	0.28	0.29
	assign (segid 3A4 and resid 409 and name N)	(segid 3A4 and resid 412 and name N)	4.83	0.22	0.23
	assign (segid 3A4 and resid 409 and name N)	(segid 3A4 and resid 412 and name O)	5.17	0.64	0.64
45	assign (segid 3A4 and resid 409 and name O)	(segid 3A4 and resid 409 and name CB)	3.10	0.09	0.09
	assign (segid 3A4 and resid 409 and name O)	(segid 3A4 and resid 409 and name CD2)	4.66	0.09	0.08
	assign (segid 3A4 and resid 409 and name O)	(segid 3A4 and resid 409 and name CG)	4.41	0.07	0.07
	assign (segid 3A4 and resid 409 and name O)	(segid 3A4 and resid 410 and name C)	3.17	0.11	0.11
	assign (segid 3A4 and resid 409 and name O)	(segid 3A4 and resid 410 and name CA)	2.76	0.03	0.03
50	assign (segid 3A4 and resid 409 and name O)	(segid 3A4 and resid 410 and name N)	2.25	0.01	0.01
	assign (segid 3A4 and resid 409 and name O)	(segid 3A4 and resid 410 and name O)	3.79	0.14	0.14
	assign (segid 3A4 and resid 409 and name O)	(segid 3A4 and resid 411 and name C)	4.67	0.27	0.26
	assign (segid 3A4 and resid 409 and name O)	(segid 3A4 and resid 411 and name CA)	4.68	0.21	0.21
	assign (segid 3A4 and resid 409 and name O)	(segid 3A4 and resid 411 and name CB)	5.80	0.29	0.29
55	assign (segid 3A4 and resid 409 and name O)	(segid 3A4 and resid 411 and name N)	3.59	0.17	0.18
	assign (segid 3A4 and resid 409 and name O)	(segid 3A4 and resid 411 and name O)	5.69	0.24	0.24
	assign (segid 3A4 and resid 409 and name O)	(segid 3A4 and resid 412 and name C)	4.16	0.28	0.29
	assign (segid 3A4 and resid 409 and name O)	(segid 3A4 and resid 412 and name CA)	4.63	0.33	0.34
	assign (segid 3A4 and resid 409 and name O)	(segid 3A4 and resid 412 and name N)	3.94	0.34	0.34
60	assign (segid 3A4 and resid 409 and name O)	(segid 3A4 and resid 412 and name O)	3.83	0.27	0.27
	assign (segid 3A4 and resid 40 and name C)	(segid 3A4 and resid 40 and name CB)	2.48	0.05	0.04
	assign (segid 3A4 and resid 40 and name C)	(segid 3A4 and resid 40 and name O)	1.23	0.00	0.00
	assign (segid 3A4 and resid 40 and name C)	(segid 3A4 and resid 41 and name C)	3.05	0.06	0.06
	assign (segid 3A4 and resid 40 and name C)	(segid 3A4 and resid 41 and name CA)	2.44	0.02	0.01
65	assign (segid 3A4 and resid 40 and name C)	(segid 3A4 and resid 41 and name CB)	3.69	0.04	0.04
	assign (segid 3A4 and resid 40 and name C)	(segid 3A4 and resid 41 and name N)	1.32	0.00	0.01
	assign (segid 3A4 and resid 40 and name C)	(segid 3A4 and resid 41 and name O)	3.86	0.08	0.08
	assign (segid 3A4 and resid 40 and name C)	(segid 3A4 and resid 42 and name C)	4.58	0.12	0.12
	assign (segid 3A4 and resid 40 and name C)	(segid 3A4 and resid 42 and name CA)	4.54	0.11	0.11
70	assign (segid 3A4 and resid 40 and name C)	(segid 3A4 and resid 42 and name CB)	5.33	0.10	0.09
	assign (segid 3A4 and resid 40 and name C)	(segid 3A4 and resid 42 and name N)	3.37	0.10	0.10
	assign (segid 3A4 and resid 40 and name C)	(segid 3A4 and resid 42 and name O)	5.56	0.26	0.25
	assign (segid 3A4 and resid 40 and name CA)	(segid 3A4 and resid 310 and name CA)	18.44	0.62	0.61
	assign (segid 3A4 and resid 40 and name CA)	(segid 3A4 and resid 310 and name CB)	18.20	0.62	0.62
75	assign (segid 3A4 and resid 40 and name CA)	(segid 3A4 and resid 313 and name CA)	17.32	0.70	0.70
	assign (segid 3A4 and resid 40 and name CA)	(segid 3A4 and resid 313 and name CB)	16.85	0.66	0.66
	assign (segid 3A4 and resid 40 and name CA)	(segid 3A4 and resid 314 and name CA)	15.30	0.69	0.69
	assign (segid 3A4 and resid 40 and name CA)	(segid 3A4 and resid 314 and name CB)	15.36	0.69	0.68
	assign (segid 3A4 and resid 40 and name CA)	(segid 3A4 and resid 315 and name CA)	18.04	0.70	0.69
80	assign (segid 3A4 and resid 40 and name CA)	(segid 3A4 and resid 317 and name CA)	15.92	0.86	0.86
	assign (segid 3A4 and resid 40 and name CA)	(segid 3A4 and resid 319 and name CA)	15.83	1.18	1.17
	assign (segid 3A4 and resid 40 and name CA)	(segid 3A4 and resid 319 and name CB)	15.30	1.31	1.32
	assign (segid 3A4 and resid 40 and name CA)	(segid 3A4 and resid 322 and name CA)	13.28	1.07	1.07

	assign	(segid 3A4 and resid 40 and name CA)	(segid 3A4 and resid 323 and name CA)	12.74	0.40	0.40
	assign	(segid 3A4 and resid 40 and name CA)	(segid 3A4 and resid 323 and name CB)	11.39	0.34	0.34
	assign	(segid 3A4 and resid 40 and name CA)	(segid 3A4 and resid 324 and name CA)	15.18	0.29	0.28
	assign	(segid 3A4 and resid 40 and name CA)	(segid 3A4 and resid 324 and name CB)	16.57	0.26	0.26
	assign	(segid 3A4 and resid 40 and name CA)	(segid 3A4 and resid 325 and name CA)	15.02	0.44	0.43
5	assign	(segid 3A4 and resid 40 and name CA)	(segid 3A4 and resid 325 and name CB)	15.13	0.43	0.43
	assign	(segid 3A4 and resid 40 and name CA)	(segid 3A4 and resid 326 and name CA)	17.29	0.56	0.56
	assign	(segid 3A4 and resid 40 and name CA)	(segid 3A4 and resid 326 and name CB)	17.05	0.62	0.62
	assign	(segid 3A4 and resid 40 and name CA)	(segid 3A4 and resid 327 and name CA)	18.32	0.60	0.59
	assign	(segid 3A4 and resid 40 and name CA)	(segid 3A4 and resid 327 and name CB)	18.32	0.62	0.61
10	assign	(segid 3A4 and resid 40 and name CA)	(segid 3A4 and resid 328 and name CA)	18.17	0.62	0.63
	assign	(segid 3A4 and resid 40 and name CA)	(segid 3A4 and resid 329 and name CA)	15.06	0.76	0.77
	assign	(segid 3A4 and resid 40 and name CA)	(segid 3A4 and resid 329 and name CB)	13.87	0.74	0.73
	assign	(segid 3A4 and resid 40 and name CA)	(segid 3A4 and resid 330 and name CA)	14.45	0.94	0.95
	assign	(segid 3A4 and resid 40 and name CA)	(segid 3A4 and resid 330 and name CB)	15.44	1.02	1.03
15	assign	(segid 3A4 and resid 40 and name CA)	(segid 3A4 and resid 331 and name CA)	11.29	0.84	0.83
	assign	(segid 3A4 and resid 40 and name CA)	(segid 3A4 and resid 331 and name CB)	10.62	0.75	0.76
	assign	(segid 3A4 and resid 40 and name CA)	(segid 3A4 and resid 332 and name CA)	11.94	1.09	1.09
	assign	(segid 3A4 and resid 40 and name CA)	(segid 3A4 and resid 332 and name CB)	15.52	1.15	1.16
	assign	(segid 3A4 and resid 40 and name CA)	(segid 3A4 and resid 333 and name CA)	15.92	0.77	0.76
20	assign	(segid 3A4 and resid 40 and name CA)	(segid 3A4 and resid 333 and name CB)	17.11	0.69	0.69
	assign	(segid 3A4 and resid 40 and name CA)	(segid 3A4 and resid 334 and name CA)	18.55	0.71	0.71
	assign	(segid 3A4 and resid 40 and name CA)	(segid 3A4 and resid 334 and name CB)	16.21	0.51	0.50
	assign	(segid 3A4 and resid 40 and name CA)	(segid 3A4 and resid 335 and name CA)	14.81	0.47	0.48
	assign	(segid 3A4 and resid 40 and name CA)	(segid 3A4 and resid 335 and name CB)	19.15	0.47	0.46
25	assign	(segid 3A4 and resid 40 and name CA)	(segid 3A4 and resid 336 and name CA)	19.46	0.39	0.38
	assign	(segid 3A4 and resid 40 and name CA)	(segid 3A4 and resid 336 and name CB)	17.93	0.37	0.37
	assign	(segid 3A4 and resid 40 and name CA)	(segid 3A4 and resid 337 and name CA)	17.42	0.40	0.41
	assign	(segid 3A4 and resid 40 and name CA)	(segid 3A4 and resid 337 and name CB)	16.29	0.32	0.32
	assign	(segid 3A4 and resid 40 and name CA)	(segid 3A4 and resid 338 and name CA)	12.94	0.20	0.20
30	assign	(segid 3A4 and resid 40 and name CA)	(segid 3A4 and resid 338 and name CB)	11.80	0.29	0.29
	assign	(segid 3A4 and resid 40 and name CA)	(segid 3A4 and resid 339 and name CA)	12.41	0.32	0.32
	assign	(segid 3A4 and resid 40 and name CA)	(segid 3A4 and resid 339 and name CB)	13.65	0.35	0.35
	assign	(segid 3A4 and resid 40 and name CA)	(segid 3A4 and resid 340 and name CA)	9.22	0.59	0.59
	assign	(segid 3A4 and resid 40 and name CA)	(segid 3A4 and resid 340 and name CB)	8.17	0.64	0.64
35	assign	(segid 3A4 and resid 40 and name CA)	(segid 3A4 and resid 341 and name CA)	10.80	0.78	0.78
	assign	(segid 3A4 and resid 40 and name CA)	(segid 3A4 and resid 341 and name CB)	11.64	0.68	0.68
	assign	(segid 3A4 and resid 40 and name CA)	(segid 3A4 and resid 342 and name CA)	9.78	0.98	0.98
	assign	(segid 3A4 and resid 40 and name CA)	(segid 3A4 and resid 342 and name CB)	10.19	1.05	1.05
	assign	(segid 3A4 and resid 40 and name CA)	(segid 3A4 and resid 343 and name CA)	12.94	0.93	0.93
40	assign	(segid 3A4 and resid 40 and name CA)	(segid 3A4 and resid 343 and name CB)	12.05	0.74	0.74
	assign	(segid 3A4 and resid 40 and name CA)	(segid 3A4 and resid 344 and name CA)	11.92	0.74	0.74
	assign	(segid 3A4 and resid 40 and name CA)	(segid 3A4 and resid 344 and name CB)	9.06	0.58	0.57
	assign	(segid 3A4 and resid 40 and name CA)	(segid 3A4 and resid 345 and name CA)	7.85	0.66	0.66
	assign	(segid 3A4 and resid 40 and name CA)	(segid 3A4 and resid 345 and name CB)	11.58	0.62	0.62
45	assign	(segid 3A4 and resid 40 and name CA)	(segid 3A4 and resid 346 and name CA)	14.07	0.50	0.49
	assign	(segid 3A4 and resid 40 and name CA)	(segid 3A4 and resid 346 and name CB)	14.95	0.54	0.54
	assign	(segid 3A4 and resid 40 and name CA)	(segid 3A4 and resid 347 and name CA)	12.52	0.37	0.37
	assign	(segid 3A4 and resid 40 and name CA)	(segid 3A4 and resid 347 and name CB)	11.11	0.40	0.40
50	assign	(segid 3A4 and resid 40 and name CA)	(segid 3A4 and resid 348 and name CA)	15.52	0.47	0.47
	assign	(segid 3A4 and resid 40 and name CA)	(segid 3A4 and resid 348 and name CB)	16.65	0.45	0.46
	assign	(segid 3A4 and resid 40 and name CA)	(segid 3A4 and resid 349 and name CA)	13.98	0.77	0.78
	assign	(segid 3A4 and resid 40 and name CA)	(segid 3A4 and resid 349 and name CB)	13.21	0.83	0.82
	assign	(segid 3A4 and resid 40 and name CA)	(segid 3A4 and resid 350 and name CA)	12.41	0.74	0.75
	assign	(segid 3A4 and resid 40 and name CA)	(segid 3A4 and resid 350 and name CB)	11.07	0.74	0.73
55	assign	(segid 3A4 and resid 40 and name CA)	(segid 3A4 and resid 351 and name CA)	15.17	0.72	0.72
	assign	(segid 3A4 and resid 40 and name CA)	(segid 3A4 and resid 351 and name CB)	14.97	0.70	0.71
	assign	(segid 3A4 and resid 40 and name CA)	(segid 3A4 and resid 352 and name CA)	18.06	0.63	0.64
	assign	(segid 3A4 and resid 40 and name CA)	(segid 3A4 and resid 352 and name CB)	16.97	0.67	0.67
60	assign	(segid 3A4 and resid 40 and name CA)	(segid 3A4 and resid 353 and name CA)	10.27	0.44	0.45
	assign	(segid 3A4 and resid 40 and name CA)	(segid 3A4 and resid 353 and name CB)	8.60	0.72	0.72
	assign	(segid 3A4 and resid 40 and name CA)	(segid 3A4 and resid 354 and name CA)	7.35	0.72	0.71
	assign	(segid 3A4 and resid 40 and name CA)	(segid 3A4 and resid 354 and name CB)	12.04	0.77	0.77
	assign	(segid 3A4 and resid 40 and name CA)	(segid 3A4 and resid 355 and name CA)	12.35	0.88	0.88
65	assign	(segid 3A4 and resid 40 and name CA)	(segid 3A4 and resid 355 and name CB)	13.03	0.86	0.86
	assign	(segid 3A4 and resid 40 and name CA)	(segid 3A4 and resid 356 and name CA)	9.23	1.07	1.06
	assign	(segid 3A4 and resid 40 and name CA)	(segid 3A4 and resid 356 and name CB)	7.10	1.16	1.16
	assign	(segid 3A4 and resid 40 and name CA)	(segid 3A4 and resid 357 and name CA)	8.35	1.24	1.25
	assign	(segid 3A4 and resid 40 and name CA)	(segid 3A4 and resid 357 and name CB)	11.88	1.25	1.25
70	assign	(segid 3A4 and resid 40 and name CA)	(segid 3A4 and resid 358 and name CA)	12.55	1.28	1.27
	assign	(segid 3A4 and resid 40 and name CA)	(segid 3A4 and resid 358 and name CB)	12.48	1.09	1.10
	assign	(segid 3A4 and resid 40 and name CA)	(segid 3A4 and resid 359 and name CA)	12.33	1.02	1.02
	assign	(segid 3A4 and resid 40 and name CA)	(segid 3A4 and resid 359 and name CB)	11.74	1.09	1.09
	assign	(segid 3A4 and resid 40 and name CA)	(segid 3A4 and resid 360 and name CA)	11.41	1.08	1.09
	assign	(segid 3A4 and resid 40 and name CA)	(segid 3A4 and resid 360 and name CB)	14.84	1.10	1.11
75	assign	(segid 3A4 and resid 40 and name CA)	(segid 3A4 and resid 361 and name CA)	15.04	1.09	1.08
	assign	(segid 3A4 and resid 40 and name CA)	(segid 3A4 and resid 361 and name CB)	16.56	0.99	0.99
	assign	(segid 3A4 and resid 40 and name CA)	(segid 3A4 and resid 362 and name CA)	1.53	0.01	0.01
	assign	(segid 3A4 and resid 40 and name CA)	(segid 3A4 and resid 362 and name CB)	1.52	0.01	0.01
	assign	(segid 3A4 and resid 40 and name CA)	(segid 3A4 and resid 363 and name CA)	2.40	0.01	0.01
80	assign	(segid 3A4 and resid 40 and name CA)	(segid 3A4 and resid 363 and name CB)	4.44	0.04	0.04
	assign	(segid 3A4 and resid 40 and name CA)	(segid 3A4 and resid 364 and name CA)	3.81	0.01	0.00
	assign	(segid 3A4 and resid 40 and name CA)	(segid 3A4 and resid 364 and name CB)	4.83	0.03	0.04

	assign (segid 3A4 and resid 40 and name CA) (segid 3A4 and resid 41 and name N)	2.42	0.00	0.01
	assign (segid 3A4 and resid 40 and name CA) (segid 3A4 and resid 41 and name O)	5.33	0.08	0.07
	assign (segid 3A4 and resid 40 and name CA) (segid 3A4 and resid 42 and name C)	5.54	0.09	0.09
	assign (segid 3A4 and resid 40 and name CA) (segid 3A4 and resid 42 and name CA)	5.55	0.09	0.09
5	assign (segid 3A4 and resid 40 and name CA) (segid 3A4 and resid 42 and name CB)	6.03	0.08	0.08
	assign (segid 3A4 and resid 40 and name CA) (segid 3A4 and resid 42 and name N)	4.48	0.08	0.07
	assign (segid 3A4 and resid 40 and name CA) (segid 3A4 and resid 42 and name O)	6.58	0.19	0.19
	assign (segid 3A4 and resid 40 and name CA) (segid 3A4 and resid 310 and name CA)	18.08	0.73	0.73
	assign (segid 3A4 and resid 40 and name CB) (segid 3A4 and resid 310 and name CB)	17.71	0.73	0.72
10	assign (segid 3A4 and resid 40 and name CB) (segid 3A4 and resid 313 and name CA)	17.34	0.80	0.81
	assign (segid 3A4 and resid 40 and name CB) (segid 3A4 and resid 313 and name CB)	16.86	0.77	0.77
	assign (segid 3A4 and resid 40 and name CB) (segid 3A4 and resid 314 and name CA)	15.15	0.79	0.80
	assign (segid 3A4 and resid 40 and name CB) (segid 3A4 and resid 314 and name CB)	15.07	0.80	0.79
	assign (segid 3A4 and resid 40 and name CB) (segid 3A4 and resid 315 and name CA)	17.97	0.79	0.78
15	assign (segid 3A4 and resid 40 and name CB) (segid 3A4 and resid 317 and name CA)	16.31	0.94	0.94
	assign (segid 3A4 and resid 40 and name CB) (segid 3A4 and resid 319 and name CA)	16.68	1.24	1.25
	assign (segid 3A4 and resid 40 and name CB) (segid 3A4 and resid 319 and name CB)	15.97	1.39	1.39
	assign (segid 3A4 and resid 40 and name CB) (segid 3A4 and resid 322 and name CA)	14.75	1.07	1.06
	assign (segid 3A4 and resid 40 and name CB) (segid 3A4 and resid 322 and name CB)	14.25	0.40	0.39
20	assign (segid 3A4 and resid 40 and name CB) (segid 3A4 and resid 323 and name CA)	12.89	0.34	0.33
	assign (segid 3A4 and resid 40 and name CB) (segid 3A4 and resid 323 and name CB)	16.66	0.30	0.29
	assign (segid 3A4 and resid 40 and name CB) (segid 3A4 and resid 324 and name CA)	18.05	0.27	0.27
	assign (segid 3A4 and resid 40 and name CB) (segid 3A4 and resid 324 and name CB)	16.38	0.47	0.46
	assign (segid 3A4 and resid 40 and name CB) (segid 3A4 and resid 325 and name CA)	16.45	0.45	0.45
	assign (segid 3A4 and resid 40 and name CB) (segid 3A4 and resid 325 and name CB)	18.57	0.61	0.60
25	assign (segid 3A4 and resid 40 and name CB) (segid 3A4 and resid 326 and name CA)	18.30	0.68	0.67
	assign (segid 3A4 and resid 40 and name CB) (segid 3A4 and resid 326 and name CB)	15.97	0.80	0.81
	assign (segid 3A4 and resid 40 and name CB) (segid 3A4 and resid 329 and name CA)	14.84	0.77	0.76
	assign (segid 3A4 and resid 40 and name CB) (segid 3A4 and resid 329 and name CB)	15.14	1.02	1.02
30	assign (segid 3A4 and resid 40 and name CB) (segid 3A4 and resid 330 and name CA)	16.03	1.12	1.11
	assign (segid 3A4 and resid 40 and name CB) (segid 3A4 and resid 330 and name CB)	11.94	0.89	0.89
	assign (segid 3A4 and resid 40 and name CB) (segid 3A4 and resid 331 and name CA)	11.42	0.80	0.81
	assign (segid 3A4 and resid 40 and name CB) (segid 3A4 and resid 331 and name CB)	12.21	1.19	1.19
	assign (segid 3A4 and resid 40 and name CB) (segid 3A4 and resid 332 and name CA)	15.82	1.28	1.29
35	assign (segid 3A4 and resid 40 and name CB) (segid 3A4 and resid 332 and name CB)	16.57	0.82	0.83
	assign (segid 3A4 and resid 40 and name CB) (segid 3A4 and resid 335 and name CA)	17.94	0.73	0.74
	assign (segid 3A4 and resid 40 and name CB) (segid 3A4 and resid 336 and name CA)	17.29	0.56	0.55
	assign (segid 3A4 and resid 40 and name CB) (segid 3A4 and resid 337 and name CA)	15.93	0.52	0.53
	assign (segid 3A4 and resid 40 and name CB) (segid 3A4 and resid 337 and name CB)	19.31	0.40	0.39
40	assign (segid 3A4 and resid 40 and name CB) (segid 3A4 and resid 341 and name CA)	18.75	0.43	0.44
	assign (segid 3A4 and resid 40 and name CB) (segid 3A4 and resid 341 and name CB)	17.75	0.33	0.32
	assign (segid 3A4 and resid 40 and name CB) (segid 3A4 and resid 342 and name CA)	14.36	0.21	0.21
	assign (segid 3A4 and resid 40 and name CB) (segid 3A4 and resid 343 and name CA)	13.22	0.30	0.30
	assign (segid 3A4 and resid 40 and name CB) (segid 3A4 and resid 343 and name CB)	13.78	0.32	0.31
45	assign (segid 3A4 and resid 40 and name CB) (segid 3A4 and resid 344 and name CA)	14.97	0.35	0.35
	assign (segid 3A4 and resid 40 and name CB) (segid 3A4 and resid 344 and name CB)	10.49	0.58	0.59
	assign (segid 3A4 and resid 40 and name CB) (segid 3A4 and resid 345 and name CA)	9.51	0.62	0.62
	assign (segid 3A4 and resid 40 and name CB) (segid 3A4 and resid 345 and name CB)	11.76	0.80	0.79
	assign (segid 3A4 and resid 40 and name CB) (segid 3A4 and resid 346 and name CA)	12.52	0.71	0.71
50	assign (segid 3A4 and resid 40 and name CB) (segid 3A4 and resid 346 and name CB)	10.49	1.03	1.03
	assign (segid 3A4 and resid 40 and name CB) (segid 3A4 and resid 347 and name CA)	10.93	1.09	1.10
	assign (segid 3A4 and resid 40 and name CB) (segid 3A4 and resid 347 and name CB)	13.41	0.98	0.98
	assign (segid 3A4 and resid 40 and name CB) (segid 3A4 and resid 348 and name CA)	12.39	0.82	0.81
	assign (segid 3A4 and resid 40 and name CB) (segid 3A4 and resid 349 and name CA)	12.36	0.80	0.81
	assign (segid 3A4 and resid 40 and name CB) (segid 3A4 and resid 349 and name CB)	9.13	0.69	0.69
55	assign (segid 3A4 and resid 40 and name CB) (segid 3A4 and resid 350 and name CA)	8.00	0.81	0.82
	assign (segid 3A4 and resid 40 and name CB) (segid 3A4 and resid 350 and name CB)	11.43	0.74	0.73
	assign (segid 3A4 and resid 40 and name CB) (segid 3A4 and resid 351 and name CA)	13.87	0.56	0.56
	assign (segid 3A4 and resid 40 and name CB) (segid 3A4 and resid 352 and name CA)	14.87	0.60	0.60
	assign (segid 3A4 and resid 40 and name CB) (segid 3A4 and resid 352 and name CB)	12.13	0.39	0.39
60	assign (segid 3A4 and resid 40 and name CB) (segid 3A4 and resid 353 and name CA)	10.68	0.40	0.39
	assign (segid 3A4 and resid 40 and name CB) (segid 3A4 and resid 353 and name CB)	14.88	0.49	0.49
	assign (segid 3A4 and resid 40 and name CB) (segid 3A4 and resid 354 and name CA)	16.05	0.48	0.48
	assign (segid 3A4 and resid 40 and name CB) (segid 3A4 and resid 354 and name CB)	13.09	0.75	0.76
	assign (segid 3A4 and resid 40 and name CB) (segid 3A4 and resid 355 and name CA)	12.34	0.78	0.78
65	assign (segid 3A4 and resid 40 and name CB) (segid 3A4 and resid 355 and name CB)	11.42	0.76	0.76
	assign (segid 3A4 and resid 40 and name CB) (segid 3A4 and resid 356 and name CA)	10.13	0.75	0.75
	assign (segid 3A4 and resid 40 and name CB) (segid 3A4 and resid 356 and name CB)	14.33	0.75	0.76
	assign (segid 3A4 and resid 40 and name CB) (segid 3A4 and resid 357 and name CA)	14.24	0.75	0.76
	assign (segid 3A4 and resid 40 and name CB) (segid 3A4 and resid 357 and name CB)	18.08	0.91	0.92
70	assign (segid 3A4 and resid 40 and name CB) (segid 3A4 and resid 358 and name CA)	17.59	0.71	0.70
	assign (segid 3A4 and resid 40 and name CB) (segid 3A4 and resid 360 and name CA)	16.53	0.74	0.74
	assign (segid 3A4 and resid 40 and name CB) (segid 3A4 and resid 360 and name CB)	9.88	0.52	0.52
	assign (segid 3A4 and resid 40 and name CB) (segid 3A4 and resid 381 and name CA)	8.74	0.87	0.87
	assign (segid 3A4 and resid 40 and name CB) (segid 3A4 and resid 382 and name CA)	7.61	0.88	0.87
75	assign (segid 3A4 and resid 40 and name CB) (segid 3A4 and resid 382 and name CB)	12.37	0.90	0.90
	assign (segid 3A4 and resid 40 and name CB) (segid 3A4 and resid 383 and name CA)	12.80	1.01	1.01
	assign (segid 3A4 and resid 40 and name CB) (segid 3A4 and resid 384 and name CA)	13.37	1.00	1.00
	assign (segid 3A4 and resid 40 and name CB) (segid 3A4 and resid 384 and name CB)	9.95	1.18	1.18
80	assign (segid 3A4 and resid 40 and name CB) (segid 3A4 and resid 385 and name CA)	7.69	1.33	1.33
	assign (segid 3A4 and resid 40 and name CB) (segid 3A4 and resid 386 and name CA)	9.02	1.33	1.33
	assign (segid 3A4 and resid 40 and name CB) (segid 3A4 and resid 387 and name CA)	12.64	1.32	1.33
	assign (segid 3A4 and resid 40 and name CB) (segid 3A4 and resid 388 and name CA)	13.36	1.32	1.32

	assign (segid 3A4 and resid 40 and name CB)	(segid 3A4 and resid 389 and name CA)	13.45	1.18	1.18
	assign (segid 3A4 and resid 40 and name CB)	(segid 3A4 and resid 389 and name CB)	13.43	1.09	1.09
	assign (segid 3A4 and resid 40 and name CB)	(segid 3A4 and resid 390 and name CA)	12.41	1.22	1.21
	assign (segid 3A4 and resid 40 and name CB)	(segid 3A4 and resid 390 and name CB)	11.92	1.21	1.21
5	assign (segid 3A4 and resid 40 and name CB)	(segid 3A4 and resid 391 and name CA)	15.48	1.23	1.22
	assign (segid 3A4 and resid 40 and name CB)	(segid 3A4 and resid 391 and name CB)	15.62	1.21	1.21
	assign (segid 3A4 and resid 40 and name CB)	(segid 3A4 and resid 394 and name CB)	16.77	1.10	1.10
	assign (segid 3A4 and resid 40 and name CB)	(segid 3A4 and resid 41 and name C)	5.42	0.05	0.06
	assign (segid 3A4 and resid 40 and name CB)	(segid 3A4 and resid 41 and name CA)	4.44	0.07	0.08
	assign (segid 3A4 and resid 40 and name CB)	(segid 3A4 and resid 41 and name CB)	5.29	0.09	0.10
10	assign (segid 3A4 and resid 40 and name CB)	(segid 3A4 and resid 41 and name N)	3.12	0.07	0.08
	assign (segid 3A4 and resid 40 and name CB)	(segid 3A4 and resid 41 and name O)	6.25	0.06	0.07
	assign (segid 3A4 and resid 40 and name CB)	(segid 3A4 and resid 42 and name C)	6.92	0.10	0.10
	assign (segid 3A4 and resid 40 and name CB)	(segid 3A4 and resid 42 and name CA)	6.88	0.07	0.07
	assign (segid 3A4 and resid 40 and name CB)	(segid 3A4 and resid 42 and name CB)	7.42	0.06	0.06
15	assign (segid 3A4 and resid 40 and name CB)	(segid 3A4 and resid 42 and name N)	5.68	0.06	0.07
	assign (segid 3A4 and resid 40 and name CB)	(segid 3A4 and resid 40 and name C)	2.45	0.02	0.01
	assign (segid 3A4 and resid 40 and name N)	(segid 3A4 and resid 40 and name CA)	1.46	0.01	0.00
	assign (segid 3A4 and resid 40 and name N)	(segid 3A4 and resid 40 and name CB)	2.47	0.02	0.01
	assign (segid 3A4 and resid 40 and name N)	(segid 3A4 and resid 40 and name O)	3.48	0.04	0.04
20	assign (segid 3A4 and resid 40 and name N)	(segid 3A4 and resid 41 and name C)	4.70	0.05	0.06
	assign (segid 3A4 and resid 40 and name N)	(segid 3A4 and resid 41 and name CA)	4.17	0.03	0.03
	assign (segid 3A4 and resid 40 and name N)	(segid 3A4 and resid 41 and name CB)	4.89	0.04	0.03
	assign (segid 3A4 and resid 40 and name N)	(segid 3A4 and resid 41 and name N)	2.77	0.03	0.03
	assign (segid 3A4 and resid 40 and name N)	(segid 3A4 and resid 41 and name O)	5.78	0.08	0.08
25	assign (segid 3A4 and resid 40 and name N)	(segid 3A4 and resid 42 and name C)	5.65	0.08	0.08
	assign (segid 3A4 and resid 40 and name N)	(segid 3A4 and resid 42 and name CA)	5.40	0.10	0.10
	assign (segid 3A4 and resid 40 and name N)	(segid 3A4 and resid 42 and name CB)	5.52	0.09	0.09
	assign (segid 3A4 and resid 40 and name N)	(segid 3A4 and resid 42 and name N)	4.38	0.08	0.08
	assign (segid 3A4 and resid 40 and name N)	(segid 3A4 and resid 42 and name O)	6.80	0.12	0.12
30	assign (segid 3A4 and resid 40 and name N)	(segid 3A4 and resid 40 and name CB)	3.27	0.07	0.07
	assign (segid 3A4 and resid 40 and name O)	(segid 3A4 and resid 41 and name C)	3.00	0.09	0.10
	assign (segid 3A4 and resid 40 and name O)	(segid 3A4 and resid 41 and name CA)	2.77	0.02	0.03
	assign (segid 3A4 and resid 40 and name O)	(segid 3A4 and resid 41 and name CB)	1.24	0.06	0.05
35	assign (segid 3A4 and resid 40 and name O)	(segid 3A4 and resid 41 and name N)	2.24	0.02	0.03
	assign (segid 3A4 and resid 40 and name O)	(segid 3A4 and resid 41 and name O)	3.45	0.10	0.10
	assign (segid 3A4 and resid 40 and name O)	(segid 3A4 and resid 42 and name C)	4.14	0.24	0.25
	assign (segid 3A4 and resid 40 and name O)	(segid 3A4 and resid 42 and name CA)	4.45	0.21	0.21
	assign (segid 3A4 and resid 40 and name O)	(segid 3A4 and resid 42 and name CB)	5.46	0.20	0.21
	assign (segid 3A4 and resid 40 and name O)	(segid 3A4 and resid 42 and name N)	3.52	0.19	0.18
40	assign (segid 3A4 and resid 40 and name O)	(segid 3A4 and resid 42 and name O)	4.95	0.40	0.39
	assign (segid 3A4 and resid 410 and name C)	(segid 3A4 and resid 410 and name O)	1.24	0.01	0.00
	assign (segid 3A4 and resid 410 and name C)	(segid 3A4 and resid 411 and name C)	3.30	0.07	0.08
	assign (segid 3A4 and resid 410 and name C)	(segid 3A4 and resid 411 and name CA)	2.44	0.03	0.02
	assign (segid 3A4 and resid 410 and name C)	(segid 3A4 and resid 411 and name CB)	3.64	0.03	0.03
45	assign (segid 3A4 and resid 410 and name C)	(segid 3A4 and resid 411 and name N)	1.33	0.01	0.01
	assign (segid 3A4 and resid 410 and name C)	(segid 3A4 and resid 411 and name O)	4.26	0.09	0.10
	assign (segid 3A4 and resid 410 and name C)	(segid 3A4 and resid 412 and name C)	5.20	0.18	0.17
	assign (segid 3A4 and resid 410 and name C)	(segid 3A4 and resid 412 and name CA)	4.89	0.11	0.11
	assign (segid 3A4 and resid 410 and name C)	(segid 3A4 and resid 412 and name N)	3.56	0.11	0.11
50	assign (segid 3A4 and resid 410 and name C)	(segid 3A4 and resid 412 and name O)	5.37	0.40	0.40
	assign (segid 3A4 and resid 410 and name CA)	(segid 3A4 and resid 410 and name C)	1.53	0.01	0.00
	assign (segid 3A4 and resid 410 and name CA)	(segid 3A4 and resid 410 and name O)	2.40	0.00	0.01
	assign (segid 3A4 and resid 410 and name CA)	(segid 3A4 and resid 411 and name C)	4.63	0.08	0.08
	assign (segid 3A4 and resid 410 and name CA)	(segid 3A4 and resid 411 and name CA)	3.80	0.02	0.01
55	assign (segid 3A4 and resid 410 and name CA)	(segid 3A4 and resid 411 and name CB)	4.77	0.03	0.03
	assign (segid 3A4 and resid 410 and name CA)	(segid 3A4 and resid 411 and name N)	2.42	0.02	0.03
	assign (segid 3A4 and resid 410 and name CA)	(segid 3A4 and resid 411 and name O)	5.68	0.11	0.11
	assign (segid 3A4 and resid 410 and name CA)	(segid 3A4 and resid 412 and name C)	5.89	0.24	0.25
	assign (segid 3A4 and resid 410 and name CA)	(segid 3A4 and resid 412 and name CA)	5.82	0.14	0.15
60	assign (segid 3A4 and resid 410 and name CA)	(segid 3A4 and resid 412 and name N)	4.58	0.12	0.12
	assign (segid 3A4 and resid 410 and name CA)	(segid 3A4 and resid 412 and name O)	5.81	0.34	0.34
	assign (segid 3A4 and resid 410 and name CA)	(segid 3A4 and resid 413 and name CA)	9.58	1.03	1.04
	assign (segid 3A4 and resid 410 and name CA)	(segid 3A4 and resid 414 and name CA)	11.39	1.62	1.62
	assign (segid 3A4 and resid 410 and name CA)	(segid 3A4 and resid 415 and name CA)	14.84	1.47	1.47
65	assign (segid 3A4 and resid 410 and name CA)	(segid 3A4 and resid 415 and name CB)	15.54	1.53	1.54
	assign (segid 3A4 and resid 410 and name CA)	(segid 3A4 and resid 440 and name CA)	16.08	0.58	0.59
	assign (segid 3A4 and resid 410 and name N)	(segid 3A4 and resid 410 and name C)	2.43	0.04	0.03
	assign (segid 3A4 and resid 410 and name N)	(segid 3A4 and resid 410 and name CA)	1.45	0.00	0.01
	assign (segid 3A4 and resid 410 and name N)	(segid 3A4 and resid 410 and name O)	3.52	0.04	0.05
70	assign (segid 3A4 and resid 410 and name N)	(segid 3A4 and resid 411 and name C)	4.75	0.12	0.12
	assign (segid 3A4 and resid 410 and name N)	(segid 3A4 and resid 411 and name CA)	4.11	0.07	0.08
	assign (segid 3A4 and resid 410 and name N)	(segid 3A4 and resid 411 and name CB)	4.89	0.12	0.12
	assign (segid 3A4 and resid 410 and name N)	(segid 3A4 and resid 411 and name N)	2.70	0.07	0.08
	assign (segid 3A4 and resid 410 and name N)	(segid 3A4 and resid 411 and name O)	5.93	0.14	0.14
75	assign (segid 3A4 and resid 410 and name N)	(segid 3A4 and resid 412 and name C)	5.52	0.31	0.31
	assign (segid 3A4 and resid 410 and name N)	(segid 3A4 and resid 412 and name CA)	5.50	0.15	0.16
	assign (segid 3A4 and resid 410 and name N)	(segid 3A4 and resid 412 and name N)	4.37	0.13	0.13
	assign (segid 3A4 and resid 410 and name N)	(segid 3A4 and resid 412 and name O)	5.27	0.18	0.19
	assign (segid 3A4 and resid 410 and name N)	(segid 3A4 and resid 411 and name C)	3.48	0.11	0.12
80	assign (segid 3A4 and resid 410 and name O)	(segid 3A4 and resid 411 and name CA)	2.79	0.06	0.06
	assign (segid 3A4 and resid 410 and name O)	(segid 3A4 and resid 411 and name CB)	4.15	0.06	0.06
	assign (segid 3A4 and resid 410 and name O)	(segid 3A4 and resid 411 and name N)	2.25	0.01	0.01

	assign (segid 3A4 and resid 410 and name O)	(segid 3A4 and resid 411 and name O)	4.16	0.14	0.13
	assign (segid 3A4 and resid 410 and name O)	(segid 3A4 and resid 412 and name C)	5.11	0.27	0.27
	assign (segid 3A4 and resid 410 and name O)	(segid 3A4 and resid 412 and name CA)	5.16	0.20	0.19
	assign (segid 3A4 and resid 410 and name O)	(segid 3A4 and resid 412 and name N)	3.95	0.19	0.19
5	assign (segid 3A4 and resid 410 and name O)	(segid 3A4 and resid 412 and name O)	5.69	0.61	0.61
	assign (segid 3A4 and resid 411 and name C)	(segid 3A4 and resid 411 and name CB)	2.48	0.03	0.03
	assign (segid 3A4 and resid 411 and name C)	(segid 3A4 and resid 411 and name O)	1.24	0.01	0.01
	assign (segid 3A4 and resid 411 and name C)	(segid 3A4 and resid 412 and name C)	3.54	0.06	0.06
	assign (segid 3A4 and resid 411 and name C)	(segid 3A4 and resid 412 and name CA)	2.44	0.02	0.01
10	assign (segid 3A4 and resid 411 and name C)	(segid 3A4 and resid 412 and name N)	1.33	0.00	0.00
	assign (segid 3A4 and resid 411 and name C)	(segid 3A4 and resid 412 and name O)	4.25	0.22	0.22
	assign (segid 3A4 and resid 411 and name CA)	(segid 3A4 and resid 411 and name C)	1.52	0.01	0.02
	assign (segid 3A4 and resid 411 and name CA)	(segid 3A4 and resid 411 and name CB)	1.53	0.01	0.00
	assign (segid 3A4 and resid 411 and name CA)	(segid 3A4 and resid 411 and name O)	2.39	0.03	0.02
15	assign (segid 3A4 and resid 411 and name CA)	(segid 3A4 and resid 412 and name C)	4.78	0.06	0.06
	assign (segid 3A4 and resid 411 and name CA)	(segid 3A4 and resid 412 and name CA)	3.81	0.01	0.02
	assign (segid 3A4 and resid 411 and name CA)	(segid 3A4 and resid 412 and name N)	2.45	0.02	0.02
	assign (segid 3A4 and resid 411 and name CA)	(segid 3A4 and resid 412 and name O)	5.29	0.25	0.25
	assign (segid 3A4 and resid 411 and name CA)	(segid 3A4 and resid 413 and name CA)	8.67	0.98	0.98
20	assign (segid 3A4 and resid 411 and name CA)	(segid 3A4 and resid 414 and name CA)	10.38	1.53	1.52
	assign (segid 3A4 and resid 411 and name CA)	(segid 3A4 and resid 415 and name CA)	13.83	1.26	1.27
	assign (segid 3A4 and resid 411 and name CA)	(segid 3A4 and resid 415 and name CB)	14.49	1.42	1.43
	assign (segid 3A4 and resid 411 and name CA)	(segid 3A4 and resid 416 and name CA)	16.58	0.90	0.90
	assign (segid 3A4 and resid 411 and name CA)	(segid 3A4 and resid 439 and name CA)	17.55	0.47	0.48
25	assign (segid 3A4 and resid 411 and name CA)	(segid 3A4 and resid 440 and name CA)	14.32	0.48	0.48
	assign (segid 3A4 and resid 411 and name CB)	(segid 3A4 and resid 412 and name C)	5.74	0.10	0.10
	assign (segid 3A4 and resid 411 and name CB)	(segid 3A4 and resid 412 and name CA)	4.55	0.04	0.04
	assign (segid 3A4 and resid 411 and name CB)	(segid 3A4 and resid 412 and name N)	3.31	0.09	0.08
	assign (segid 3A4 and resid 411 and name CB)	(segid 3A4 and resid 412 and name O)	6.23	0.12	0.12
30	assign (segid 3A4 and resid 411 and name CB)	(segid 3A4 and resid 413 and name CA)	9.54	0.86	0.86
	assign (segid 3A4 and resid 411 and name CB)	(segid 3A4 and resid 414 and name CA)	10.84	1.53	1.54
	assign (segid 3A4 and resid 411 and name CB)	(segid 3A4 and resid 415 and name CA)	14.20	1.22	1.23
	assign (segid 3A4 and resid 411 and name CB)	(segid 3A4 and resid 415 and name CB)	14.92	1.34	1.35
	assign (segid 3A4 and resid 411 and name CB)	(segid 3A4 and resid 416 and name CA)	16.74	0.92	0.93
35	assign (segid 3A4 and resid 411 and name CB)	(segid 3A4 and resid 439 and name CA)	17.20	0.58	0.59
	assign (segid 3A4 and resid 411 and name CB)	(segid 3A4 and resid 440 and name CA)	14.15	0.57	0.57
	assign (segid 3A4 and resid 411 and name N)	(segid 3A4 and resid 411 and name C)	2.48	0.03	0.03
	assign (segid 3A4 and resid 411 and name N)	(segid 3A4 and resid 411 and name CA)	1.45	0.01	0.01
	assign (segid 3A4 and resid 411 and name N)	(segid 3A4 and resid 411 and name CB)	2.45	0.02	0.03
40	assign (segid 3A4 and resid 411 and name N)	(segid 3A4 and resid 411 and name O)	3.58	0.04	0.04
	assign (segid 3A4 and resid 411 and name N)	(segid 3A4 and resid 412 and name C)	4.86	0.14	0.13
	assign (segid 3A4 and resid 411 and name N)	(segid 3A4 and resid 412 and name CA)	4.23	0.05	0.05
	assign (segid 3A4 and resid 411 and name N)	(segid 3A4 and resid 412 and name N)	2.79	0.03	0.04
	assign (segid 3A4 and resid 411 and name N)	(segid 3A4 and resid 412 and name O)	5.11	0.27	0.27
45	assign (segid 3A4 and resid 411 and name O)	(segid 3A4 and resid 411 and name CB)	3.10	0.12	0.12
	assign (segid 3A4 and resid 411 and name O)	(segid 3A4 and resid 412 and name C)	3.93	0.12	0.12
	assign (segid 3A4 and resid 411 and name O)	(segid 3A4 and resid 412 and name CA)	2.77	0.04	0.05
	assign (segid 3A4 and resid 411 and name O)	(segid 3A4 and resid 412 and name N)	2.25	0.02	0.02
	assign (segid 3A4 and resid 411 and name O)	(segid 3A4 and resid 412 and name O)	4.84	0.22	0.21
50	assign (segid 3A4 and resid 412 and name C)	(segid 3A4 and resid 412 and name O)	1.23	0.01	0.00
	assign (segid 3A4 and resid 412 and name C)	(segid 3A4 and resid 413 and name C)	4.71	1.19	1.19
	assign (segid 3A4 and resid 412 and name C)	(segid 3A4 and resid 413 and name CA)	4.08	1.08	1.08
	assign (segid 3A4 and resid 412 and name C)	(segid 3A4 and resid 413 and name N)	2.96	1.16	1.15
	assign (segid 3A4 and resid 412 and name C)	(segid 3A4 and resid 413 and name O)	5.22	1.17	1.17
55	assign (segid 3A4 and resid 412 and name CA)	(segid 3A4 and resid 412 and name C)	1.51	0.00	0.01
	assign (segid 3A4 and resid 412 and name CA)	(segid 3A4 and resid 412 and name O)	2.40	0.02	0.01
	assign (segid 3A4 and resid 412 and name CA)	(segid 3A4 and resid 413 and name CA)	5.07	0.87	0.87
	assign (segid 3A4 and resid 412 and name CA)	(segid 3A4 and resid 413 and name N)	3.98	1.10	1.09
	assign (segid 3A4 and resid 412 and name CA)	(segid 3A4 and resid 413 and name O)	6.72	1.49	1.49
60	assign (segid 3A4 and resid 412 and name CA)	(segid 3A4 and resid 414 and name CA)	10.19	1.26	1.27
	assign (segid 3A4 and resid 412 and name CA)	(segid 3A4 and resid 415 and name CB)	10.80	1.47	1.46
	assign (segid 3A4 and resid 412 and name CA)	(segid 3A4 and resid 416 and name CA)	13.10	0.87	0.87
	assign (segid 3A4 and resid 412 and name CA)	(segid 3A4 and resid 417 and name CA)	15.30	1.17	1.16
	assign (segid 3A4 and resid 412 and name CA)	(segid 3A4 and resid 438 and name CA)	16.19	0.56	0.56
65	assign (segid 3A4 and resid 412 and name CA)	(segid 3A4 and resid 439 and name CA)	14.70	0.45	0.44
	assign (segid 3A4 and resid 412 and name CA)	(segid 3A4 and resid 440 and name CA)	11.20	0.47	0.46
	assign (segid 3A4 and resid 412 and name N)	(segid 3A4 and resid 412 and name C)	2.45	0.04	0.04
	assign (segid 3A4 and resid 412 and name N)	(segid 3A4 and resid 412 and name CA)	1.46	0.01	0.00
	assign (segid 3A4 and resid 412 and name N)	(segid 3A4 and resid 412 and name O)	3.04	0.18	0.18
70	assign (segid 3A4 and resid 412 and name N)	(segid 3A4 and resid 413 and name N)	5.24	1.13	1.13
	assign (segid 3A4 and resid 412 and name N)	(segid 3A4 and resid 413 and name O)	4.69	1.00	1.01
	assign (segid 3A4 and resid 412 and name O)	(segid 3A4 and resid 413 and name CA)	4.12	0.87	0.88
	assign (segid 3A4 and resid 412 and name O)	(segid 3A4 and resid 413 and name N)	3.29	0.80	0.80
	assign (segid 3A4 and resid 412 and name O)	(segid 3A4 and resid 413 and name O)	5.32	0.77	0.77
75	assign (segid 3A4 and resid 412 and name O)	(segid 3A4 and resid 414 and name N)	4.88	1.50	1.49
	assign (segid 3A4 and resid 413 and name C)	(segid 3A4 and resid 413 and name O)	1.23	0.00	0.01
	assign (segid 3A4 and resid 413 and name C)	(segid 3A4 and resid 414 and name C)	3.33	0.19	0.19
	assign (segid 3A4 and resid 413 and name C)	(segid 3A4 and resid 414 and name CA)	2.44	0.02	0.01
	assign (segid 3A4 and resid 413 and name C)	(segid 3A4 and resid 414 and name N)	1.32	0.01	0.01
80	assign (segid 3A4 and resid 413 and name C)	(segid 3A4 and resid 414 and name O)	3.73	0.24	0.24
	assign (segid 3A4 and resid 413 and name C)	(segid 3A4 and resid 415 and name C)	6.53	0.20	0.20
	assign (segid 3A4 and resid 413 and name C)	(segid 3A4 and resid 415 and name CA)	5.43	0.33	0.33
	assign (segid 3A4 and resid 413 and name C)	(segid 3A4 and resid 415 and name CB)	5.79	0.61	0.60

	assign (segid 3A4 and resid 413 and name C) (segid 3A4 and resid 415 and name N)	4.22	0.27	0.28
	assign (segid 3A4 and resid 413 and name C) (segid 3A4 and resid 415 and name O)	6.66	0.18	0.17
	assign (segid 3A4 and resid 413 and name CA) (segid 3A4 and resid 413 and name C)	1.52	0.01	0.02
	assign (segid 3A4 and resid 413 and name CA) (segid 3A4 and resid 413 and name O)	2.39	0.02	0.02
5	assign (segid 3A4 and resid 413 and name CA) (segid 3A4 and resid 414 and name C)	4.61	0.11	0.10
	assign (segid 3A4 and resid 413 and name CA) (segid 3A4 and resid 414 and name CA)	3.81	0.02	0.02
	assign (segid 3A4 and resid 413 and name CA) (segid 3A4 and resid 414 and name N)	2.43	0.01	0.02
	assign (segid 3A4 and resid 413 and name CA) (segid 3A4 and resid 414 and name O)	4.73	0.17	0.16
	assign (segid 3A4 and resid 413 and name CA) (segid 3A4 and resid 415 and name CA)	6.68	0.24	0.24
	assign (segid 3A4 and resid 413 and name CA) (segid 3A4 and resid 415 and name CB)	6.94	0.60	0.60
10	assign (segid 3A4 and resid 413 and name CA) (segid 3A4 and resid 415 and name N)	5.59	0.21	0.20
	assign (segid 3A4 and resid 413 and name CA) (segid 3A4 and resid 416 and name CA)	10.03	0.36	0.37
	assign (segid 3A4 and resid 413 and name CA) (segid 3A4 and resid 417 and name CA)	12.12	0.43	0.44
	assign (segid 3A4 and resid 413 and name CA) (segid 3A4 and resid 424 and name CA)	18.53	1.08	1.09
	assign (segid 3A4 and resid 413 and name CA) (segid 3A4 and resid 437 and name CA)	18.72	1.10	1.10
15	assign (segid 3A4 and resid 413 and name CA) (segid 3A4 and resid 438 and name CA)	15.13	1.18	1.18
	assign (segid 3A4 and resid 413 and name CA) (segid 3A4 and resid 439 and name CA)	13.36	1.06	1.05
	assign (segid 3A4 and resid 413 and name CA) (segid 3A4 and resid 440 and name CA)	9.64	1.07	1.07
	assign (segid 3A4 and resid 413 and name N) (segid 3A4 and resid 413 and name C)	2.41	0.09	0.09
	assign (segid 3A4 and resid 413 and name N) (segid 3A4 and resid 413 and name CA)	1.46	0.01	0.01
20	assign (segid 3A4 and resid 413 and name N) (segid 3A4 and resid 413 and name O)	2.96	0.39	0.39
	assign (segid 3A4 and resid 413 and name N) (segid 3A4 and resid 414 and name C)	5.57	0.32	0.32
	assign (segid 3A4 and resid 413 and name N) (segid 3A4 and resid 414 and name CA)	4.54	0.26	0.25
	assign (segid 3A4 and resid 413 and name N) (segid 3A4 and resid 414 and name N)	3.25	0.33	0.33
	assign (segid 3A4 and resid 413 and name N) (segid 3A4 and resid 414 and name O)	5.78	0.39	0.40
25	assign (segid 3A4 and resid 413 and name N) (segid 3A4 and resid 415 and name N)	6.53	0.35	0.34
	assign (segid 3A4 and resid 413 and name N) (segid 3A4 and resid 414 and name C)	3.57	0.40	0.41
	assign (segid 3A4 and resid 413 and name O) (segid 3A4 and resid 414 and name CA)	2.78	0.04	0.03
	assign (segid 3A4 and resid 413 and name O) (segid 3A4 and resid 414 and name N)	2.24	0.01	0.02
30	assign (segid 3A4 and resid 413 and name O) (segid 3A4 and resid 414 and name O)	4.20	0.48	0.48
	assign (segid 3A4 and resid 413 and name O) (segid 3A4 and resid 415 and name C)	6.37	0.52	0.53
	assign (segid 3A4 and resid 413 and name O) (segid 3A4 and resid 415 and name CA)	5.33	0.67	0.67
	assign (segid 3A4 and resid 413 and name O) (segid 3A4 and resid 415 and name CB)	5.52	0.97	0.97
	assign (segid 3A4 and resid 413 and name O) (segid 3A4 and resid 415 and name N)	4.13	0.53	0.54
35	assign (segid 3A4 and resid 413 and name O) (segid 3A4 and resid 415 and name O)	6.38	0.41	0.42
	assign (segid 3A4 and resid 413 and name O) (segid 3A4 and resid 440 and name C)	7.62	0.06	0.06
	assign (segid 3A4 and resid 414 and name C) (segid 3A4 and resid 414 and name O)	1.24	0.01	0.00
	assign (segid 3A4 and resid 414 and name C) (segid 3A4 and resid 415 and name C)	3.49	0.18	0.18
40	assign (segid 3A4 and resid 414 and name C) (segid 3A4 and resid 415 and name CA)	2.43	0.01	0.01
	assign (segid 3A4 and resid 414 and name C) (segid 3A4 and resid 415 and name CB)	3.40	0.15	0.15
	assign (segid 3A4 and resid 414 and name C) (segid 3A4 and resid 415 and name N)	1.34	0.02	0.01
	assign (segid 3A4 and resid 414 and name C) (segid 3A4 and resid 415 and name O)	3.89	0.23	0.22
	assign (segid 3A4 and resid 414 and name C) (segid 3A4 and resid 416 and name C)	6.48	0.23	0.24
	assign (segid 3A4 and resid 414 and name C) (segid 3A4 and resid 416 and name CA)	5.68	0.29	0.28
45	assign (segid 3A4 and resid 414 and name C) (segid 3A4 and resid 416 and name N)	4.42	0.24	0.24
	assign (segid 3A4 and resid 414 and name C) (segid 3A4 and resid 416 and name O)	6.76	0.33	0.33
	assign (segid 3A4 and resid 414 and name C) (segid 3A4 and resid 417 and name N)	7.20	0.40	0.39
	assign (segid 3A4 and resid 414 and name C) (segid 3A4 and resid 440 and name C)	6.24	0.56	0.55
	assign (segid 3A4 and resid 414 and name C) (segid 3A4 and resid 440 and name CA)	6.19	0.67	0.67
	assign (segid 3A4 and resid 414 and name C) (segid 3A4 and resid 440 and name O)	7.34	0.52	0.52
50	assign (segid 3A4 and resid 414 and name CA) (segid 3A4 and resid 414 and name C)	1.52	0.01	0.01
	assign (segid 3A4 and resid 414 and name CA) (segid 3A4 and resid 414 and name O)	2.40	0.03	0.02
	assign (segid 3A4 and resid 414 and name CA) (segid 3A4 and resid 415 and name C)	4.68	0.15	0.15
	assign (segid 3A4 and resid 414 and name CA) (segid 3A4 and resid 415 and name CA)	3.79	0.01	0.02
	assign (segid 3A4 and resid 414 and name CA) (segid 3A4 and resid 415 and name CB)	4.66	0.08	0.08
55	assign (segid 3A4 and resid 414 and name CA) (segid 3A4 and resid 415 and name N)	2.43	0.02	0.01
	assign (segid 3A4 and resid 414 and name CA) (segid 3A4 and resid 415 and name O)	4.77	0.23	0.22
	assign (segid 3A4 and resid 414 and name CA) (segid 3A4 and resid 416 and name C)	7.64	0.24	0.24
	assign (segid 3A4 and resid 414 and name CA) (segid 3A4 and resid 416 and name CA)	6.85	0.25	0.26
60	assign (segid 3A4 and resid 414 and name CA) (segid 3A4 and resid 416 and name N)	5.72	0.22	0.21
	assign (segid 3A4 and resid 414 and name CA) (segid 3A4 and resid 417 and name CA)	9.22	0.41	0.42
	assign (segid 3A4 and resid 414 and name CA) (segid 3A4 and resid 423 and name CA)	14.82	2.08	2.08
	assign (segid 3A4 and resid 414 and name CA) (segid 3A4 and resid 424 and name CA)	15.04	1.13	1.12
	assign (segid 3A4 and resid 414 and name CA) (segid 3A4 and resid 425 and name CA)	17.22	1.98	1.98
65	assign (segid 3A4 and resid 414 and name CA) (segid 3A4 and resid 435 and name CA)	16.87	0.50	0.49
	assign (segid 3A4 and resid 414 and name CA) (segid 3A4 and resid 436 and name CA)	17.77	0.53	0.54
	assign (segid 3A4 and resid 414 and name CA) (segid 3A4 and resid 437 and name CA)	15.29	0.62	0.63
	assign (segid 3A4 and resid 414 and name CA) (segid 3A4 and resid 438 and name CA)	11.72	0.69	0.68
	assign (segid 3A4 and resid 414 and name CA) (segid 3A4 and resid 439 and name CA)	10.13	0.58	0.57
70	assign (segid 3A4 and resid 414 and name CA) (segid 3A4 and resid 440 and name C)	6.49	0.29	0.29
	assign (segid 3A4 and resid 414 and name CA) (segid 3A4 and resid 440 and name CA)	6.60	0.40	0.40
	assign (segid 3A4 and resid 414 and name CA) (segid 3A4 and resid 440 and name O)	7.48	0.21	0.22
	assign (segid 3A4 and resid 414 and name N) (segid 3A4 and resid 414 and name CA)	2.44	0.03	0.03
	assign (segid 3A4 and resid 414 and name N) (segid 3A4 and resid 414 and name O)	1.46	0.01	0.00
	assign (segid 3A4 and resid 414 and name N) (segid 3A4 and resid 415 and name C)	2.80	0.09	0.10
75	assign (segid 3A4 and resid 414 and name N) (segid 3A4 and resid 415 and name CA)	5.82	0.20	0.20
	assign (segid 3A4 and resid 414 and name N) (segid 3A4 and resid 415 and name CB)	4.78	0.05	0.05
	assign (segid 3A4 and resid 414 and name N) (segid 3A4 and resid 415 and name N)	5.42	0.26	0.25
	assign (segid 3A4 and resid 414 and name N) (segid 3A4 and resid 415 and name O)	3.54	0.05	0.06
80	assign (segid 3A4 and resid 414 and name N) (segid 3A4 and resid 415 and name O)	6.01	0.28	0.27
	assign (segid 3A4 and resid 414 and name N) (segid 3A4 and resid 416 and name N)	6.80	0.30	0.29
	assign (segid 3A4 and resid 414 and name O) (segid 3A4 and resid 415 and name C)	3.90	0.29	0.30
	assign (segid 3A4 and resid 414 and name O) (segid 3A4 and resid 415 and name CA)	2.76	0.03	0.03

5	assign	(segid 3A4 and resid 414 and name O)	(segid 3A4 and resid 415 and name CB)	3.67	0.26	0.25
	assign	(segid 3A4 and resid 414 and name O)	(segid 3A4 and resid 415 and name N)	2.25	0.01	0.01
	assign	(segid 3A4 and resid 414 and name O)	(segid 3A4 and resid 415 and name O)	4.58	0.32	0.31
	assign	(segid 3A4 and resid 411 and name O)	(segid 3A4 and resid 416 and name C)	6.76	0.39	0.39
	assign	(segid 3A4 and resid 414 and name O)	(segid 3A4 and resid 416 and name CA)	5.85	0.49	0.48
10	assign	(segid 3A4 and resid 414 and name O)	(segid 3A4 and resid 416 and name N)	4.53	0.40	0.41
	assign	(segid 3A4 and resid 414 and name O)	(segid 3A4 and resid 416 and name O)	6.99	0.35	0.34
	assign	(segid 3A4 and resid 414 and name O)	(segid 3A4 and resid 416 and name C)	6.93	1.25	1.25
	assign	(segid 3A4 and resid 414 and name O)	(segid 3A4 and resid 440 and name CA)	6.79	1.31	1.31
	assign	(segid 3A4 and resid 414 and name O)	(segid 3A4 and resid 415 and name CB)	2.51	0.04	0.04
15	assign	(segid 3A4 and resid 415 and name C)	(segid 3A4 and resid 415 and name O)	1.24	0.01	0.00
	assign	(segid 3A4 and resid 415 and name C)	(segid 3A4 and resid 416 and name C)	3.05	0.06	0.07
	assign	(segid 3A4 and resid 415 and name C)	(segid 3A4 and resid 416 and name CA)	2.42	0.01	0.01
	assign	(segid 3A4 and resid 415 and name C)	(segid 3A4 and resid 416 and name N)	1.32	0.01	0.01
	assign	(segid 3A4 and resid 415 and name C)	(segid 3A4 and resid 416 and name O)	3.44	0.32	0.31
20	assign	(segid 3A4 and resid 415 and name C)	(segid 3A4 and resid 417 and name C)	6.09	0.28	0.27
	assign	(segid 3A4 and resid 415 and name C)	(segid 3A4 and resid 417 and name CA)	4.97	0.29	0.28
	assign	(segid 3A4 and resid 415 and name C)	(segid 3A4 and resid 417 and name N)	3.85	0.32	0.31
	assign	(segid 3A4 and resid 415 and name C)	(segid 3A4 and resid 417 and name O)	7.02	0.41	0.42
	assign	(segid 3A4 and resid 415 and name C)	(segid 3A4 and resid 439 and name C)	5.84	0.48	0.48
25	assign	(segid 3A4 and resid 415 and name C)	(segid 3A4 and resid 439 and name O)	5.07	0.60	0.61
	assign	(segid 3A4 and resid 415 and name C)	(segid 3A4 and resid 440 and name C)	4.92	0.13	0.12
	assign	(segid 3A4 and resid 415 and name C)	(segid 3A4 and resid 440 and name CA)	4.57	0.19	0.19
	assign	(segid 3A4 and resid 415 and name C)	(segid 3A4 and resid 440 and name N)	5.69	0.28	0.27
	assign	(segid 3A4 and resid 415 and name C)	(segid 3A4 and resid 440 and name O)	6.08	0.11	0.11
30	assign	(segid 3A4 and resid 415 and name C)	(segid 3A4 and resid 440 and name O)	1.52	0.01	0.02
	assign	(segid 3A4 and resid 415 and name CA)	(segid 3A4 and resid 415 and name C)	1.54	0.02	0.01
	assign	(segid 3A4 and resid 415 and name CA)	(segid 3A4 and resid 415 and name CB)	2.40	0.02	0.01
	assign	(segid 3A4 and resid 415 and name CA)	(segid 3A4 and resid 416 and name C)	4.38	0.03	0.04
	assign	(segid 3A4 and resid 415 and name CA)	(segid 3A4 and resid 416 and name CA)	3.78	0.01	0.02
35	assign	(segid 3A4 and resid 415 and name CA)	(segid 3A4 and resid 416 and name N)	2.41	0.02	0.02
	assign	(segid 3A4 and resid 415 and name CA)	(segid 3A4 and resid 416 and name O)	4.51	0.32	0.33
	assign	(segid 3A4 and resid 415 and name CA)	(segid 3A4 and resid 416 and name C)	7.34	0.30	0.30
	assign	(segid 3A4 and resid 415 and name CA)	(segid 3A4 and resid 417 and name C)	6.23	0.37	0.36
	assign	(segid 3A4 and resid 415 and name CA)	(segid 3A4 and resid 417 and name N)	5.23	0.36	0.36
40	assign	(segid 3A4 and resid 415 and name CA)	(segid 3A4 and resid 417 and name CA)	11.93	2.29	2.29
	assign	(segid 3A4 and resid 415 and name CA)	(segid 3A4 and resid 423 and name CA)	12.59	1.70	1.70
	assign	(segid 3A4 and resid 415 and name CA)	(segid 3A4 and resid 424 and name CA)	15.08	2.57	2.58
	assign	(segid 3A4 and resid 415 and name CA)	(segid 3A4 and resid 425 and name CA)	15.67	1.13	1.12
	assign	(segid 3A4 and resid 415 and name CA)	(segid 3A4 and resid 435 and name CA)	16.37	1.02	1.02
45	assign	(segid 3A4 and resid 415 and name CA)	(segid 3A4 and resid 436 and name CA)	13.72	1.18	1.18
	assign	(segid 3A4 and resid 415 and name CA)	(segid 3A4 and resid 437 and name CA)	10.12	1.16	1.17
	assign	(segid 3A4 and resid 415 and name CA)	(segid 3A4 and resid 438 and name CA)	6.96	0.91	0.91
	assign	(segid 3A4 and resid 415 and name CA)	(segid 3A4 and resid 439 and name C)	8.41	0.98	0.99
	assign	(segid 3A4 and resid 415 and name CA)	(segid 3A4 and resid 439 and name O)	6.24	1.08	1.08
50	assign	(segid 3A4 and resid 415 and name CA)	(segid 3A4 and resid 439 and name CA)	5.71	0.21	0.21
	assign	(segid 3A4 and resid 415 and name CA)	(segid 3A4 and resid 440 and name C)	5.48	0.40	0.40
	assign	(segid 3A4 and resid 415 and name CA)	(segid 3A4 and resid 440 and name CA)	6.69	0.65	0.65
	assign	(segid 3A4 and resid 415 and name CA)	(segid 3A4 and resid 440 and name N)	6.86	0.24	0.24
	assign	(segid 3A4 and resid 415 and name CA)	(segid 3A4 and resid 440 and name O)	6.86	0.09	0.09
55	assign	(segid 3A4 and resid 415 and name CB)	(segid 3A4 and resid 416 and name C)	4.52	0.10	0.09
	assign	(segid 3A4 and resid 415 and name CB)	(segid 3A4 and resid 416 and name N)	3.23	0.11	0.11
	assign	(segid 3A4 and resid 415 and name CB)	(segid 3A4 and resid 416 and name O)	4.46	0.44	0.45
	assign	(segid 3A4 and resid 415 and name CB)	(segid 3A4 and resid 417 and name C)	7.32	0.37	0.37
	assign	(segid 3A4 and resid 415 and name CB)	(segid 3A4 and resid 417 and name CA)	6.24	0.50	0.50
60	assign	(segid 3A4 and resid 415 and name CB)	(segid 3A4 and resid 417 and name N)	5.53	0.45	0.46
	assign	(segid 3A4 and resid 415 and name CB)	(segid 3A4 and resid 417 and name O)	12.30	2.61	2.61
	assign	(segid 3A4 and resid 415 and name CB)	(segid 3A4 and resid 423 and name CA)	13.12	2.29	2.29
	assign	(segid 3A4 and resid 415 and name CB)	(segid 3A4 and resid 424 and name CA)	16.54	1.70	1.70
	assign	(segid 3A4 and resid 415 and name CB)	(segid 3A4 and resid 435 and name CA)	17.20	1.58	1.57
65	assign	(segid 3A4 and resid 415 and name CB)	(segid 3A4 and resid 436 and name CA)	14.50	1.59	1.58
	assign	(segid 3A4 and resid 415 and name CB)	(segid 3A4 and resid 437 and name CA)	10.98	1.50	1.50
	assign	(segid 3A4 and resid 415 and name CB)	(segid 3A4 and resid 438 and name CA)	9.14	1.08	1.08
	assign	(segid 3A4 and resid 415 and name CB)	(segid 3A4 and resid 439 and name C)	6.44	0.15	0.15
	assign	(segid 3A4 and resid 415 and name CB)	(segid 3A4 and resid 440 and name CA)	6.38	0.27	0.28
70	assign	(segid 3A4 and resid 415 and name CB)	(segid 3A4 and resid 440 and name O)	7.51	0.18	0.17
	assign	(segid 3A4 and resid 415 and name CB)	(segid 3A4 and resid 440 and name C)	2.43	0.04	0.04
	assign	(segid 3A4 and resid 415 and name N)	(segid 3A4 and resid 415 and name CA)	1.46	0.01	0.00
	assign	(segid 3A4 and resid 415 and name N)	(segid 3A4 and resid 415 and name CB)	2.47	0.02	0.01
	assign	(segid 3A4 and resid 415 and name N)	(segid 3A4 and resid 415 and name O)	2.74	0.08	0.09
75	assign	(segid 3A4 and resid 415 and name N)	(segid 3A4 and resid 416 and name C)	5.43	0.08	0.08
	assign	(segid 3A4 and resid 415 and name N)	(segid 3A4 and resid 416 and name CA)	4.78	0.06	0.06
	assign	(segid 3A4 and resid 415 and name N)	(segid 3A4 and resid 416 and name N)	3.55	0.06	0.06
	assign	(segid 3A4 and resid 415 and name N)	(segid 3A4 and resid 416 and name O)	5.68	0.34	0.34
	assign	(segid 3A4 and resid 415 and name N)	(segid 3A4 and resid 417 and name CA)	7.11	0.36	0.36
80	assign	(segid 3A4 and resid 415 and name N)	(segid 3A4 and resid 417 and name N)	6.12	0.35	0.36
	assign	(segid 3A4 and resid 415 and name N)	(segid 3A4 and resid 417 and name O)	7.25	0.62	0.63
	assign	(segid 3A4 and resid 415 and name N)	(segid 3A4 and resid 439 and name C)	6.72	0.81	0.81
	assign	(segid 3A4 and resid 415 and name N)	(segid 3A4 and resid 439 and name O)	5.49	0.12	0.12
	assign	(segid 3A4 and resid 415 and name N)	(segid 3A4 and resid 440 and name CA)	5.43	0.24	0.25
80	assign	(segid 3A4 and resid 415 and name N)	(segid 3A4 and resid 440 and name N)	6.76	0.40	0.40
	assign	(segid 3A4 and resid 415 and name N)	(segid 3A4 and resid 440 and name O)	6.62	0.10	0.10
	assign	(segid 3A4 and resid 415 and name O)	(segid 3A4 and resid 415 and name CB)	3.22	0.09	0.09

601

	assign (segid 3A4 and resid 417 and name CA)	(segid 3A4 and resid 436 and name CA)	15.16	0.66	0.67
	assign (segid 3A4 and resid 417 and name CA)	(segid 3A4 and resid 437 and name CA)	12.08	0.84	0.84
	assign (segid 3A4 and resid 417 and name CA)	(segid 3A4 and resid 438 and name CA)	9.25	1.11	1.11
	assign (segid 3A4 and resid 417 and name CA)	(segid 3A4 and resid 439 and name CA)	6.69	1.19	1.19
5	assign (segid 3A4 and resid 417 and name CA)	(segid 3A4 and resid 439 and name O)	5.06	1.22	1.21
	assign (segid 3A4 and resid 417 and name CA)	(segid 3A4 and resid 440 and name CA)	6.02	1.21	1.21
	assign (segid 3A4 and resid 417 and name N)	(segid 3A4 and resid 417 and name C)	2.45	0.04	0.04
	assign (segid 3A4 and resid 417 and name N)	(segid 3A4 and resid 417 and name CA)	1.46	0.01	0.00
	assign (segid 3A4 and resid 417 and name N)	(segid 3A4 and resid 417 and name O)	3.47	0.22	0.21
10	assign (segid 3A4 and resid 417 and name N)	(segid 3A4 and resid 439 and name C)	5.02	1.07	1.08
	assign (segid 3A4 and resid 417 and name N)	(segid 3A4 and resid 439 and name CA)	6.07	0.99	0.99
	assign (segid 3A4 and resid 417 and name N)	(segid 3A4 and resid 439 and name O)	4.11	1.13	1.13
	assign (segid 3A4 and resid 417 and name N)	(segid 3A4 and resid 440 and name C)	5.50	0.85	0.85
	assign (segid 3A4 and resid 417 and name N)	(segid 3A4 and resid 440 and name CA)	5.08	1.03	1.03
15	assign (segid 3A4 and resid 417 and name N)	(segid 3A4 and resid 440 and name N)	5.47	1.02	1.02
	assign (segid 3A4 and resid 417 and name N)	(segid 3A4 and resid 440 and name O)	6.29	0.84	0.85
	assign (segid 3A4 and resid 417 and name O)	(segid 3A4 and resid 439 and name O)	6.44	0.84	0.84
	assign (segid 3A4 and resid 41 and name C)	(segid 3A4 and resid 41 and name CB)	2.46	0.04	0.04
	assign (segid 3A4 and resid 41 and name C)	(segid 3A4 and resid 41 and name O)	1.23	0.01	0.01
20	assign (segid 3A4 and resid 41 and name C)	(segid 3A4 and resid 42 and name C)	3.01	0.04	0.04
	assign (segid 3A4 and resid 41 and name C)	(segid 3A4 and resid 42 and name CA)	2.42	0.00	0.01
	assign (segid 3A4 and resid 41 and name C)	(segid 3A4 and resid 42 and name CB)	3.69	0.03	0.02
	assign (segid 3A4 and resid 41 and name C)	(segid 3A4 and resid 42 and name N)	1.32	0.01	0.02
	assign (segid 3A4 and resid 41 and name C)	(segid 3A4 and resid 42 and name O)	3.78	0.17	0.18
25	assign (segid 3A4 and resid 41 and name CA)	(segid 3A4 and resid 322 and name CA)	13.73	1.26	1.26
	assign (segid 3A4 and resid 41 and name CA)	(segid 3A4 and resid 323 and name CA)	12.26	0.83	0.82
	assign (segid 3A4 and resid 41 and name CA)	(segid 3A4 and resid 323 and name CB)	10.80	0.81	0.80
	assign (segid 3A4 and resid 41 and name CA)	(segid 3A4 and resid 324 and name CA)	13.85	0.69	0.68
	assign (segid 3A4 and resid 41 and name CA)	(segid 3A4 and resid 324 and name CB)	15.28	0.69	0.69
30	assign (segid 3A4 and resid 41 and name CA)	(segid 3A4 and resid 325 and name CA)	12.83	0.76	0.76
	assign (segid 3A4 and resid 41 and name CA)	(segid 3A4 and resid 325 and name CB)	12.76	0.71	0.70
	assign (segid 3A4 and resid 41 and name CA)	(segid 3A4 and resid 326 and name CA)	14.89	0.84	0.85
	assign (segid 3A4 and resid 41 and name CA)	(segid 3A4 and resid 326 and name CB)	14.71	0.92	0.91
	assign (segid 3A4 and resid 41 and name CA)	(segid 3A4 and resid 327 and name CA)	15.37	0.95	0.94
35	assign (segid 3A4 and resid 41 and name CA)	(segid 3A4 and resid 327 and name CB)	15.26	0.92	0.92
	assign (segid 3A4 and resid 41 and name CA)	(segid 3A4 and resid 328 and name CA)	14.97	0.85	0.85
	assign (segid 3A4 and resid 41 and name CA)	(segid 3A4 and resid 328 and name CB)	16.13	0.85	0.86
	assign (segid 3A4 and resid 41 and name CA)	(segid 3A4 and resid 329 and name CA)	11.69	0.90	0.90
	assign (segid 3A4 and resid 41 and name CA)	(segid 3A4 and resid 329 and name CB)	10.57	0.87	0.88
40	assign (segid 3A4 and resid 41 and name CA)	(segid 3A4 and resid 330 and name CA)	11.06	1.00	1.01
	assign (segid 3A4 and resid 41 and name CA)	(segid 3A4 and resid 330 and name CB)	12.00	1.05	1.04
	assign (segid 3A4 and resid 41 and name CA)	(segid 3A4 and resid 331 and name CA)	8.25	0.79	0.79
	assign (segid 3A4 and resid 41 and name CA)	(segid 3A4 and resid 331 and name CB)	7.81	0.68	0.67
	assign (segid 3A4 and resid 41 and name CA)	(segid 3A4 and resid 332 and name CA)	9.42	0.95	0.95
45	assign (segid 3A4 and resid 41 and name CA)	(segid 3A4 and resid 333 and name CA)	12.76	1.12	1.12
	assign (segid 3A4 and resid 41 and name CA)	(segid 3A4 and resid 335 and name CA)	13.27	0.75	0.76
	assign (segid 3A4 and resid 41 and name CA)	(segid 3A4 and resid 336 and name CA)	14.12	0.81	0.80
	assign (segid 3A4 and resid 41 and name CA)	(segid 3A4 and resid 336 and name CB)	15.48	0.81	0.81
	assign (segid 3A4 and resid 41 and name CA)	(segid 3A4 and resid 337 and name CA)	13.48	0.70	0.71
50	assign (segid 3A4 and resid 41 and name CA)	(segid 3A4 and resid 337 and name CB)	12.17	0.71	0.71
	assign (segid 3A4 and resid 41 and name CA)	(segid 3A4 and resid 338 and name CA)	16.40	0.77	0.77
	assign (segid 3A4 and resid 41 and name CA)	(segid 3A4 and resid 338 and name CB)	17.74	0.75	0.76
	assign (segid 3A4 and resid 41 and name CA)	(segid 3A4 and resid 339 and name CA)	16.82	0.75	0.75
	assign (segid 3A4 and resid 41 and name CA)	(segid 3A4 and resid 339 and name CB)	17.83	0.74	0.74
55	assign (segid 3A4 and resid 41 and name CA)	(segid 3A4 and resid 340 and name CA)	17.68	0.83	0.84
	assign (segid 3A4 and resid 41 and name CA)	(segid 3A4 and resid 341 and name CA)	16.09	0.73	0.73
	assign (segid 3A4 and resid 41 and name CA)	(segid 3A4 and resid 341 and name CB)	15.45	0.70	0.69
	assign (segid 3A4 and resid 41 and name CA)	(segid 3A4 and resid 342 and name CA)	15.20	0.71	0.71
	assign (segid 3A4 and resid 41 and name CA)	(segid 3A4 and resid 343 and name CA)	12.21	0.55	0.55
60	assign (segid 3A4 and resid 41 and name CA)	(segid 3A4 and resid 343 and name CB)	10.84	0.61	0.61
	assign (segid 3A4 and resid 41 and name CA)	(segid 3A4 and resid 344 and name CA)	12.79	0.45	0.45
	assign (segid 3A4 and resid 41 and name CA)	(segid 3A4 and resid 344 and name CB)	14.14	0.44	0.44
	assign (segid 3A4 and resid 41 and name CA)	(segid 3A4 and resid 345 and name CA)	10.38	0.62	0.61
	assign (segid 3A4 and resid 41 and name CA)	(segid 3A4 and resid 345 and name CB)	9.40	0.75	0.75
65	assign (segid 3A4 and resid 41 and name CA)	(segid 3A4 and resid 346 and name CA)	12.76	0.61	0.61
	assign (segid 3A4 and resid 41 and name CA)	(segid 3A4 and resid 346 and name CB)	13.45	0.46	0.46
	assign (segid 3A4 and resid 41 and name CA)	(segid 3A4 and resid 347 and name CA)	12.66	0.79	0.79
	assign (segid 3A4 and resid 41 and name CA)	(segid 3A4 and resid 347 and name CB)	13.17	0.86	0.86
	assign (segid 3A4 and resid 41 and name CA)	(segid 3A4 and resid 348 and name CA)	15.87	0.75	0.74
70	assign (segid 3A4 and resid 41 and name CA)	(segid 3A4 and resid 349 and name CA)	14.56	0.57	0.57
	assign (segid 3A4 and resid 41 and name CA)	(segid 3A4 and resid 349 and name CB)	14.10	0.58	0.59
	assign (segid 3A4 and resid 41 and name CA)	(segid 3A4 and resid 350 and name CA)	11.95	0.48	0.49
	assign (segid 3A4 and resid 41 and name CA)	(segid 3A4 and resid 350 and name CB)	10.89	0.56	0.56
	assign (segid 3A4 and resid 41 and name CA)	(segid 3A4 and resid 351 and name CA)	14.93	0.57	0.56
75	assign (segid 3A4 and resid 41 and name CA)	(segid 3A4 and resid 352 and name CA)	17.02	0.47	0.47
	assign (segid 3A4 and resid 41 and name CA)	(segid 3A4 and resid 352 and name CB)	17.82	0.49	0.48
	assign (segid 3A4 and resid 41 and name CA)	(segid 3A4 and resid 353 and name CA)	15.03	0.43	0.43
	assign (segid 3A4 and resid 41 and name CA)	(segid 3A4 and resid 353 and name CB)	13.57	0.49	0.50
	assign (segid 3A4 and resid 41 and name CA)	(segid 3A4 and resid 354 and name CA)	17.83	0.54	0.54
80	assign (segid 3A4 and resid 41 and name CA)	(segid 3A4 and resid 354 and name CB)	18.79	0.53	0.54
	assign (segid 3A4 and resid 41 and name CA)	(segid 3A4 and resid 355 and name CA)	15.94	0.90	0.89
	assign (segid 3A4 and resid 41 and name CA)	(segid 3A4 and resid 355 and name CB)	14.89	0.95	0.96
	assign (segid 3A4 and resid 41 and name CA)	(segid 3A4 and resid 356 and name CA)	15.04	0.81	0.81

	assign (segid 3A4 and resid 41 and name CA) (segid 3A4 and resid 356 and name CB)	13.85	0.79	0.78
	assign (segid 3A4 and resid 41 and name CA) (segid 3A4 and resid 357 and name CA)	18.15	0.75	0.75
	assign (segid 3A4 and resid 41 and name CA) (segid 3A4 and resid 357 and name CB)	18.11	0.73	0.72
	assign (segid 3A4 and resid 41 and name CA) (segid 3A4 and resid 381 and name CA)	14.00	0.44	0.44
5	assign (segid 3A4 and resid 41 and name CA) (segid 3A4 and resid 382 and name CA)	12.24	0.58	0.58
	assign (segid 3A4 and resid 41 and name CA) (segid 3A4 and resid 382 and name CB)	10.93	0.55	0.54
	assign (segid 3A4 and resid 41 and name CA) (segid 3A4 and resid 383 and name CA)	15.55	0.59	0.58
	assign (segid 3A4 and resid 41 and name CA) (segid 3A4 and resid 384 and name CA)	15.56	0.64	0.65
	assign (segid 3A4 and resid 41 and name CA) (segid 3A4 and resid 384 and name CB)	16.26	0.64	0.64
10	assign (segid 3A4 and resid 41 and name CA) (segid 3A4 and resid 385 and name CA)	12.12	0.74	0.75
	assign (segid 3A4 and resid 41 and name CA) (segid 3A4 and resid 386 and name CA)	9.67	0.83	0.83
	assign (segid 3A4 and resid 41 and name CA) (segid 3A4 and resid 387 and name CA)	9.65	1.16	1.16
	assign (segid 3A4 and resid 41 and name CA) (segid 3A4 and resid 388 and name CA)	12.66	1.22	1.21
	assign (segid 3A4 and resid 41 and name CA) (segid 3A4 and resid 388 and name CB)	12.90	1.27	1.26
15	assign (segid 3A4 and resid 41 and name CA) (segid 3A4 and resid 389 and name CA)	13.78	0.88	0.88
	assign (segid 3A4 and resid 41 and name CA) (segid 3A4 and resid 389 and name CB)	13.47	0.79	0.78
	assign (segid 3A4 and resid 41 and name CA) (segid 3A4 and resid 390 and name CA)	13.95	0.87	0.87
	assign (segid 3A4 and resid 41 and name CA) (segid 3A4 and resid 390 and name CB)	13.71	0.90	0.89
	assign (segid 3A4 and resid 41 and name CA) (segid 3A4 and resid 391 and name CA)	17.37	0.88	0.88
20	assign (segid 3A4 and resid 41 and name CA) (segid 3A4 and resid 391 and name CB)	17.79	0.86	0.86
	assign (segid 3A4 and resid 41 and name CA) (segid 3A4 and resid 41 and name C)	1.52	0.02	0.01
	assign (segid 3A4 and resid 41 and name CA) (segid 3A4 and resid 41 and name CB)	1.51	0.02	0.02
	assign (segid 3A4 and resid 41 and name CA) (segid 3A4 and resid 41 and name O)	2.39	0.02	0.01
25	assign (segid 3A4 and resid 41 and name CA) (segid 3A4 and resid 42 and name C)	4.39	0.05	0.05
	assign (segid 3A4 and resid 41 and name CA) (segid 3A4 and resid 42 and name CA)	3.80	0.01	0.01
	assign (segid 3A4 and resid 41 and name CA) (segid 3A4 and resid 42 and name CB)	4.83	0.04	0.03
	assign (segid 3A4 and resid 41 and name CA) (segid 3A4 and resid 42 and name N)	2.43	0.02	0.02
	assign (segid 3A4 and resid 41 and name CA) (segid 3A4 and resid 42 and name O)	5.23	0.20	0.19
30	assign (segid 3A4 and resid 41 and name CB) (segid 3A4 and resid 322 and name CA)	14.33	1.27	1.27
	assign (segid 3A4 and resid 41 and name CB) (segid 3A4 and resid 323 and name CA)	12.82	0.90	0.89
	assign (segid 3A4 and resid 41 and name CB) (segid 3A4 and resid 323 and name CB)	11.37	0.87	0.88
	assign (segid 3A4 and resid 41 and name CB) (segid 3A4 and resid 324 and name CA)	14.15	0.79	0.80
	assign (segid 3A4 and resid 41 and name CB) (segid 3A4 and resid 324 and name CB)	15.62	0.79	0.80
35	assign (segid 3A4 and resid 41 and name CB) (segid 3A4 and resid 325 and name CA)	12.90	0.87	0.86
	assign (segid 3A4 and resid 41 and name CB) (segid 3A4 and resid 325 and name CB)	12.65	0.81	0.81
	assign (segid 3A4 and resid 41 and name CB) (segid 3A4 and resid 326 and name CA)	15.08	0.93	0.93
	assign (segid 3A4 and resid 41 and name CB) (segid 3A4 and resid 326 and name CB)	15.01	1.00	1.00
	assign (segid 3A4 and resid 41 and name CB) (segid 3A4 and resid 327 and name CA)	15.22	1.06	1.07
40	assign (segid 3A4 and resid 41 and name CB) (segid 3A4 and resid 327 and name CB)	15.13	1.03	1.04
	assign (segid 3A4 and resid 41 and name CB) (segid 3A4 and resid 328 and name CA)	14.47	0.95	0.96
	assign (segid 3A4 and resid 41 and name CB) (segid 3A4 and resid 328 and name CB)	15.55	0.96	0.96
	assign (segid 3A4 and resid 41 and name CB) (segid 3A4 and resid 329 and name CA)	11.04	0.99	0.99
	assign (segid 3A4 and resid 41 and name CB) (segid 3A4 and resid 329 and name CB)	10.05	0.96	0.96
45	assign (segid 3A4 and resid 41 and name CB) (segid 3A4 and resid 330 and name CA)	10.01	1.11	1.11
	assign (segid 3A4 and resid 41 and name CB) (segid 3A4 and resid 330 and name CB)	10.88	1.16	1.16
	assign (segid 3A4 and resid 41 and name CB) (segid 3A4 and resid 331 and name CA)	7.05	0.88	0.88
	assign (segid 3A4 and resid 41 and name CB) (segid 3A4 and resid 331 and name CB)	6.74	0.77	0.77
	assign (segid 3A4 and resid 41 and name CB) (segid 3A4 and resid 332 and name CA)	8.01	0.95	0.94
50	assign (segid 3A4 and resid 41 and name CB) (segid 3A4 and resid 333 and name CA)	11.36	1.12	1.12
	assign (segid 3A4 and resid 41 and name CB) (segid 3A4 and resid 335 and name CA)	12.03	0.81	0.80
	assign (segid 3A4 and resid 41 and name CB) (segid 3A4 and resid 336 and name CA)	13.07	0.88	0.88
	assign (segid 3A4 and resid 41 and name CB) (segid 3A4 and resid 336 and name CB)	14.41	0.89	0.89
	assign (segid 3A4 and resid 41 and name CB) (segid 3A4 and resid 337 and name CA)	12.74	0.82	0.83
55	assign (segid 3A4 and resid 41 and name CB) (segid 3A4 and resid 337 and name CB)	11.50	0.82	0.83
	assign (segid 3A4 and resid 41 and name CB) (segid 3A4 and resid 338 and name CA)	15.84	0.89	0.89
	assign (segid 3A4 and resid 41 and name CB) (segid 3A4 and resid 338 and name CB)	17.16	0.87	0.87
	assign (segid 3A4 and resid 41 and name CB) (segid 3A4 and resid 339 and name CA)	16.56	0.87	0.88
	assign (segid 3A4 and resid 41 and name CB) (segid 3A4 and resid 339 and name CB)	17.60	0.87	0.86
60	assign (segid 3A4 and resid 41 and name CB) (segid 3A4 and resid 340 and name CA)	17.62	0.93	0.94
	assign (segid 3A4 and resid 41 and name CB) (segid 3A4 and resid 341 and name CA)	15.88	0.84	0.85
	assign (segid 3A4 and resid 41 and name CB) (segid 3A4 and resid 341 and name CB)	15.12	0.81	0.80
	assign (segid 3A4 and resid 41 and name CB) (segid 3A4 and resid 342 and name CA)	15.21	0.82	0.82
	assign (segid 3A4 and resid 41 and name CB) (segid 3A4 and resid 343 and name CA)	12.23	0.65	0.65
65	assign (segid 3A4 and resid 41 and name CB) (segid 3A4 and resid 343 and name CB)	10.85	0.71	0.72
	assign (segid 3A4 and resid 41 and name CB) (segid 3A4 and resid 344 and name CA)	12.99	0.49	0.48
	assign (segid 3A4 and resid 41 and name CB) (segid 3A4 and resid 344 and name CB)	14.28	0.47	0.47
	assign (segid 3A4 and resid 41 and name CB) (segid 3A4 and resid 345 and name CA)	10.73	0.60	0.61
	assign (segid 3A4 and resid 41 and name CB) (segid 3A4 and resid 345 and name CB)	9.92	0.76	0.75
	assign (segid 3A4 and resid 41 and name CB) (segid 3A4 and resid 346 and name CA)	13.07	0.55	0.54
70	assign (segid 3A4 and resid 41 and name CB) (segid 3A4 and resid 346 and name CB)	13.61	0.42	0.42
	assign (segid 3A4 and resid 41 and name CB) (segid 3A4 and resid 347 and name CA)	13.27	0.71	0.72
	assign (segid 3A4 and resid 41 and name CB) (segid 3A4 and resid 347 and name CB)	13.92	0.78	0.78
	assign (segid 3A4 and resid 41 and name CB) (segid 3A4 and resid 348 and name CA)	16.30	0.67	0.67
75	assign (segid 3A4 and resid 41 and name CB) (segid 3A4 and resid 349 and name CA)	14.66	0.53	0.54
	assign (segid 3A4 and resid 41 and name CB) (segid 3A4 and resid 349 and name CB)	14.11	0.58	0.57
	assign (segid 3A4 and resid 41 and name CB) (segid 3A4 and resid 350 and name CA)	12.20	0.47	0.47
	assign (segid 3A4 and resid 41 and name CB) (segid 3A4 and resid 350 and name CB)	11.27	0.55	0.56
	assign (segid 3A4 and resid 41 and name CB) (segid 3A4 and resid 351 and name CA)	15.34	0.56	0.56
80	assign (segid 3A4 and resid 41 and name CB) (segid 3A4 and resid 352 and name CA)	17.14	0.47	0.47
	assign (segid 3A4 and resid 41 and name CB) (segid 3A4 and resid 352 and name CB)	17.92	0.46	0.46
	assign (segid 3A4 and resid 41 and name CB) (segid 3A4 and resid 353 and name CA)	14.91	0.46	0.45
	assign (segid 3A4 and resid 41 and name CB) (segid 3A4 and resid 353 and name CB)	13.45	0.53	0.53
	assign (segid 3A4 and resid 41 and name CB) (segid 3A4 and resid 354 and name CA)	17.57	0.57	0.58

	assign (segid 3A4 and resid 41 and name CB) (segid 3A4 and resid 354 and name CB)	18.45	0.58	0.57
	assign (segid 3A4 and resid 41 and name CB) (segid 3A4 and resid 355 and name CA)	15.58	0.95	0.96
	assign (segid 3A4 and resid 41 and name CB) (segid 3A4 and resid 355 and name CB)	14.45	1.03	1.02
	assign (segid 3A4 and resid 41 and name CB) (segid 3A4 and resid 356 and name CA)	15.04	0.85	0.85
5	assign (segid 3A4 and resid 41 and name CB) (segid 3A4 and resid 356 and name CB)	13.94	0.82	0.82
	assign (segid 3A4 and resid 41 and name CB) (segid 3A4 and resid 357 and name CB)	18.30	0.73	0.74
	assign (segid 3A4 and resid 41 and name CB) (segid 3A4 and resid 381 and name CA)	14.83	0.43	0.44
	assign (segid 3A4 and resid 41 and name CB) (segid 3A4 and resid 382 and name CA)	13.24	0.58	0.58
	assign (segid 3A4 and resid 41 and name CB) (segid 3A4 and resid 382 and name CB)	11.88	0.54	0.54
10	assign (segid 3A4 and resid 41 and name CB) (segid 3A4 and resid 383 and name CA)	16.56	0.56	0.56
	assign (segid 3A4 and resid 41 and name CB) (segid 3A4 and resid 384 and name CA)	16.80	0.61	0.62
	assign (segid 3A4 and resid 41 and name CB) (segid 3A4 and resid 384 and name CB)	17.54	0.63	0.62
	assign (segid 3A4 and resid 41 and name CB) (segid 3A4 and resid 385 and name CA)	13.38	0.71	0.70
	assign (segid 3A4 and resid 41 and name CB) (segid 3A4 and resid 386 and name CA)	11.07	0.80	0.79
15	assign (segid 3A4 and resid 41 and name CB) (segid 3A4 and resid 387 and name CA)	11.13	1.13	1.12
	assign (segid 3A4 and resid 41 and name CB) (segid 3A4 and resid 388 and name CA)	14.09	1.17	1.18
	assign (segid 3A4 and resid 41 and name CB) (segid 3A4 and resid 388 and name CB)	14.29	1.24	1.23
	assign (segid 3A4 and resid 41 and name CB) (segid 3A4 and resid 389 and name CA)	15.18	0.81	0.80
	assign (segid 3A4 and resid 41 and name CB) (segid 3A4 and resid 389 and name CB)	14.80	0.70	0.70
20	assign (segid 3A4 and resid 41 and name CB) (segid 3A4 and resid 390 and name CA)	15.38	0.81	0.82
	assign (segid 3A4 and resid 41 and name CB) (segid 3A4 and resid 390 and name CB)	15.16	0.86	0.85
	assign (segid 3A4 and resid 41 and name CB) (segid 3A4 and resid 42 and name C)	5.36	0.06	0.05
	assign (segid 3A4 and resid 41 and name CB) (segid 3A4 and resid 42 and name CA)	4.39	0.04	0.05
	assign (segid 3A4 and resid 41 and name CB) (segid 3A4 and resid 42 and name CB)	5.20	0.06	0.06
25	assign (segid 3A4 and resid 41 and name CB) (segid 3A4 and resid 42 and name N)	3.07	0.04	0.04
	assign (segid 3A4 and resid 41 and name CB) (segid 3A4 and resid 42 and name O)	6.17	0.14	0.14
	assign (segid 3A4 and resid 41 and name CB) (segid 3A4 and resid 41 and name C)	2.47	0.03	0.03
	assign (segid 3A4 and resid 41 and name N) (segid 3A4 and resid 41 and name CA)	1.46	0.01	0.01
	assign (segid 3A4 and resid 41 and name N) (segid 3A4 and resid 41 and name CB)	2.44	0.04	0.04
30	assign (segid 3A4 and resid 41 and name N) (segid 3A4 and resid 41 and name O)	3.49	0.04	0.04
	assign (segid 3A4 and resid 41 and name N) (segid 3A4 and resid 42 and name C)	4.69	0.05	0.04
	assign (segid 3A4 and resid 41 and name N) (segid 3A4 and resid 42 and name CA)	4.24	0.05	0.04
	assign (segid 3A4 and resid 41 and name N) (segid 3A4 and resid 42 and name CB)	5.00	0.05	0.04
	assign (segid 3A4 and resid 41 and name N) (segid 3A4 and resid 42 and name N)	2.85	0.04	0.04
35	assign (segid 3A4 and resid 41 and name N) (segid 3A4 and resid 42 and name O)	5.69	0.17	0.18
	assign (segid 3A4 and resid 41 and name O) (segid 3A4 and resid 41 and name CB)	3.27	0.04	0.05
	assign (segid 3A4 and resid 41 and name O) (segid 3A4 and resid 42 and name C)	2.99	0.06	0.06
	assign (segid 3A4 and resid 41 and name O) (segid 3A4 and resid 42 and name CA)	2.76	0.04	0.04
	assign (segid 3A4 and resid 41 and name O) (segid 3A4 and resid 42 and name CB)	4.23	0.03	0.03
40	assign (segid 3A4 and resid 41 and name O) (segid 3A4 and resid 42 and name N)	2.24	0.01	0.01
	assign (segid 3A4 and resid 41 and name O) (segid 3A4 and resid 42 and name O)	3.39	0.20	0.19
	assign (segid 3A4 and resid 423 and name C) (segid 3A4 and resid 423 and name O)	1.24	0.01	0.00
	assign (segid 3A4 and resid 423 and name C) (segid 3A4 and resid 424 and name C)	3.17	0.16	0.17
45	assign (segid 3A4 and resid 423 and name C) (segid 3A4 and resid 424 and name CA)	2.43	0.03	0.02
	assign (segid 3A4 and resid 423 and name C) (segid 3A4 and resid 424 and name N)	1.32	0.01	0.01
	assign (segid 3A4 and resid 423 and name C) (segid 3A4 and resid 425 and name C)	3.69	0.44	0.44
	assign (segid 3A4 and resid 423 and name C) (segid 3A4 and resid 425 and name CA)	5.01	0.12	0.12
	assign (segid 3A4 and resid 423 and name C) (segid 3A4 and resid 425 and name N)	3.83	0.14	0.14
50	assign (segid 3A4 and resid 423 and name C) (segid 3A4 and resid 425 and name O)	6.52	0.49	0.49
	assign (segid 3A4 and resid 423 and name C) (segid 3A4 and resid 426 and name N)	6.76	0.20	0.20
	assign (segid 3A4 and resid 423 and name C) (segid 3A4 and resid 437 and name O)	6.88	0.79	0.78
	assign (segid 3A4 and resid 423 and name CA) (segid 3A4 and resid 423 and name C)	1.53	0.01	0.01
	assign (segid 3A4 and resid 423 and name CA) (segid 3A4 and resid 423 and name O)	2.40	0.01	0.01
55	assign (segid 3A4 and resid 423 and name CA) (segid 3A4 and resid 424 and name C)	4.46	0.09	0.08
	assign (segid 3A4 and resid 423 and name CA) (segid 3A4 and resid 424 and name CA)	3.80	0.04	0.04
	assign (segid 3A4 and resid 423 and name CA) (segid 3A4 and resid 424 and name N)	2.42	0.04	0.04
	assign (segid 3A4 and resid 423 and name CA) (segid 3A4 and resid 424 and name O)	4.74	0.46	0.46
	assign (segid 3A4 and resid 423 and name CA) (segid 3A4 and resid 425 and name C)	7.26	0.34	0.34
60	assign (segid 3A4 and resid 423 and name CA) (segid 3A4 and resid 425 and name CA)	6.16	0.22	0.21
	assign (segid 3A4 and resid 423 and name CA) (segid 3A4 and resid 425 and name N)	5.12	0.29	0.29
	assign (segid 3A4 and resid 423 and name CA) (segid 3A4 and resid 426 and name CA)	9.06	0.25	0.24
	assign (segid 3A4 and resid 423 and name CA) (segid 3A4 and resid 427 and name CA)	12.25	0.55	0.55
	assign (segid 3A4 and resid 423 and name CA) (segid 3A4 and resid 428 and name CA)	14.57	0.60	0.60
65	assign (segid 3A4 and resid 423 and name CA) (segid 3A4 and resid 429 and name CA)	17.34	1.25	1.26
	assign (segid 3A4 and resid 423 and name CA) (segid 3A4 and resid 433 and name CA)	16.25	1.39	1.39
	assign (segid 3A4 and resid 423 and name CA) (segid 3A4 and resid 434 and name CA)	13.89	1.07	1.06
	assign (segid 3A4 and resid 423 and name CA) (segid 3A4 and resid 435 and name CA)	10.67	1.04	1.04
	assign (segid 3A4 and resid 423 and name CA) (segid 3A4 and resid 436 and name CA)	10.62	1.62	1.62
70	assign (segid 3A4 and resid 423 and name CA) (segid 3A4 and resid 437 and name CA)	9.33	0.93	0.93
	assign (segid 3A4 and resid 423 and name CA) (segid 3A4 and resid 438 and name CA)	8.37	1.06	1.05
	assign (segid 3A4 and resid 423 and name CA) (segid 3A4 and resid 439 and name CA)	9.12	1.61	1.60
	assign (segid 3A4 and resid 423 and name CA) (segid 3A4 and resid 440 and name CA)	11.06	1.69	1.68
	assign (segid 3A4 and resid 423 and name N) (segid 3A4 and resid 423 and name C)	2.48	0.05	0.06
75	assign (segid 3A4 and resid 423 and name N) (segid 3A4 and resid 423 and name CA)	1.46	0.01	0.01
	assign (segid 3A4 and resid 423 and name N) (segid 3A4 and resid 423 and name O)	3.12	0.33	0.33
	assign (segid 3A4 and resid 423 and name N) (segid 3A4 and resid 424 and name C)	5.44	0.30	0.31
	assign (segid 3A4 and resid 423 and name N) (segid 3A4 and resid 424 and name CA)	4.60	0.24	0.24
	assign (segid 3A4 and resid 423 and name N) (segid 3A4 and resid 424 and name N)	3.26	0.30	0.31
80	assign (segid 3A4 and resid 423 and name N) (segid 3A4 and resid 424 and name O)	5.74	0.65	0.65
	assign (segid 3A4 and resid 423 and name N) (segid 3A4 and resid 425 and name CA)	7.25	0.17	0.16
	assign (segid 3A4 and resid 423 and name N) (segid 3A4 and resid 425 and name N)	6.15	0.20	0.20
	assign (segid 3A4 and resid 423 and name O) (segid 3A4 and resid 424 and name C)	3.36	0.36	0.35

	assign	(segid 3A4 and resid 423 and name O)	(segid 3A4 and resid 424 and name CA)	2.78	0.04	0.03
	assign	(segid 3A4 and resid 423 and name O)	(segid 3A4 and resid 424 and name N)	2.25	0.02	0.03
	assign	(segid 3A4 and resid 423 and name O)	(segid 3A4 and resid 424 and name O)	4.03	0.57	0.57
	assign	(segid 3A4 and resid 423 and name O)	(segid 3A4 and resid 425 and name C)	5.98	0.30	0.29
5	assign	(segid 3A4 and resid 423 and name O)	(segid 3A4 and resid 425 and name CA)	4.85	0.41	0.41
	assign	(segid 3A4 and resid 423 and name O)	(segid 3A4 and resid 425 and name N)	3.72	0.27	0.28
	assign	(segid 3A4 and resid 423 and name O)	(segid 3A4 and resid 425 and name O)	6.33	0.42	0.43
	assign	(segid 3A4 and resid 423 and name O)	(segid 3A4 and resid 426 and name N)	6.79	0.39	0.38
	assign	(segid 3A4 and resid 423 and name O)	(segid 3A4 and resid 426 and name O)	1.23	0.00	0.00
10	assign	(segid 3A4 and resid 424 and name C)	(segid 3A4 and resid 425 and name C)	3.19	0.07	0.07
	assign	(segid 3A4 and resid 424 and name C)	(segid 3A4 and resid 425 and name CA)	2.45	0.01	0.01
	assign	(segid 3A4 and resid 424 and name C)	(segid 3A4 and resid 425 and name N)	1.33	0.01	0.01
	assign	(segid 3A4 and resid 424 and name C)	(segid 3A4 and resid 425 and name O)	3.76	0.20	0.20
	assign	(segid 3A4 and resid 424 and name C)	(segid 3A4 and resid 426 and name C)	6.22	0.16	0.16
15	assign	(segid 3A4 and resid 424 and name C)	(segid 3A4 and resid 426 and name CA)	5.02	0.14	0.14
	assign	(segid 3A4 and resid 424 and name C)	(segid 3A4 and resid 426 and name N)	3.83	0.15	0.15
	assign	(segid 3A4 and resid 424 and name C)	(segid 3A4 and resid 426 and name O)	6.46	0.22	0.22
	assign	(segid 3A4 and resid 424 and name C)	(segid 3A4 and resid 427 and name N)	7.21	0.12	0.13
	assign	(segid 3A4 and resid 424 and name C)	(segid 3A4 and resid 427 and name O)	1.53	0.00	0.00
20	assign	(segid 3A4 and resid 424 and name CA)	(segid 3A4 and resid 424 and name C)	2.40	0.01	0.00
	assign	(segid 3A4 and resid 424 and name CA)	(segid 3A4 and resid 425 and name C)	4.54	0.04	0.03
	assign	(segid 3A4 and resid 424 and name CA)	(segid 3A4 and resid 425 and name CA)	3.83	0.02	0.01
	assign	(segid 3A4 and resid 424 and name CA)	(segid 3A4 and resid 425 and name N)	2.45	0.03	0.02
	assign	(segid 3A4 and resid 424 and name CA)	(segid 3A4 and resid 425 and name O)	4.85	0.20	0.20
25	assign	(segid 3A4 and resid 424 and name CA)	(segid 3A4 and resid 426 and name C)	7.58	0.14	0.14
	assign	(segid 3A4 and resid 424 and name CA)	(segid 3A4 and resid 426 and name CA)	6.31	0.13	0.13
	assign	(segid 3A4 and resid 424 and name CA)	(segid 3A4 and resid 426 and name N)	5.24	0.15	0.16
	assign	(segid 3A4 and resid 424 and name CA)	(segid 3A4 and resid 427 and name CA)	9.79	0.11	0.11
	assign	(segid 3A4 and resid 424 and name CA)	(segid 3A4 and resid 428 and name CA)	12.47	0.34	0.34
30	assign	(segid 3A4 and resid 424 and name CA)	(segid 3A4 and resid 429 and name CA)	15.12	0.89	0.89
	assign	(segid 3A4 and resid 424 and name CA)	(segid 3A4 and resid 430 and name CA)	18.10	0.98	0.98
	assign	(segid 3A4 and resid 424 and name CA)	(segid 3A4 and resid 433 and name CA)	13.54	1.66	1.66
	assign	(segid 3A4 and resid 424 and name CA)	(segid 3A4 and resid 434 and name CA)	11.27	1.47	1.47
	assign	(segid 3A4 and resid 424 and name CA)	(segid 3A4 and resid 435 and name CA)	8.03	1.33	1.34
35	assign	(segid 3A4 and resid 424 and name CA)	(segid 3A4 and resid 436 and name CA)	8.54	1.13	1.12
	assign	(segid 3A4 and resid 424 and name CA)	(segid 3A4 and resid 437 and name CA)	7.99	1.03	1.02
	assign	(segid 3A4 and resid 424 and name CA)	(segid 3A4 and resid 438 and name CA)	7.44	1.28	1.28
	assign	(segid 3A4 and resid 424 and name CA)	(segid 3A4 and resid 439 and name CA)	9.40	1.45	1.44
	assign	(segid 3A4 and resid 424 and name CA)	(segid 3A4 and resid 440 and name CA)	11.50	1.15	1.15
40	assign	(segid 3A4 and resid 424 and name N)	(segid 3A4 and resid 424 and name C)	2.43	0.02	0.01
	assign	(segid 3A4 and resid 424 and name N)	(segid 3A4 and resid 424 and name CA)	1.46	0.02	0.01
	assign	(segid 3A4 and resid 424 and name N)	(segid 3A4 and resid 424 and name O)	2.95	0.24	0.23
	assign	(segid 3A4 and resid 424 and name N)	(segid 3A4 and resid 425 and name C)	5.51	0.24	0.23
	assign	(segid 3A4 and resid 424 and name N)	(segid 3A4 and resid 425 and name CA)	4.61	0.21	0.22
45	assign	(segid 3A4 and resid 424 and name N)	(segid 3A4 and resid 425 and name N)	3.33	0.27	0.28
	assign	(segid 3A4 and resid 424 and name N)	(segid 3A4 and resid 425 and name O)	5.95	0.43	0.43
	assign	(segid 3A4 and resid 424 and name N)	(segid 3A4 and resid 426 and name CA)	7.26	0.18	0.17
	assign	(segid 3A4 and resid 424 and name N)	(segid 3A4 and resid 426 and name N)	6.12	0.16	0.16
	assign	(segid 3A4 and resid 424 and name N)	(segid 3A4 and resid 426 and name O)	3.33	0.19	0.19
50	assign	(segid 3A4 and resid 424 and name O)	(segid 3A4 and resid 425 and name C)	2.78	0.04	0.04
	assign	(segid 3A4 and resid 424 and name O)	(segid 3A4 and resid 425 and name N)	2.25	0.03	0.02
	assign	(segid 3A4 and resid 424 and name O)	(segid 3A4 and resid 425 and name O)	4.12	0.33	0.32
	assign	(segid 3A4 and resid 424 and name O)	(segid 3A4 and resid 426 and name C)	5.91	0.30	0.30
	assign	(segid 3A4 and resid 424 and name O)	(segid 3A4 and resid 426 and name CA)	4.69	0.29	0.28
55	assign	(segid 3A4 and resid 424 and name O)	(segid 3A4 and resid 426 and name N)	3.55	0.23	0.23
	assign	(segid 3A4 and resid 424 and name O)	(segid 3A4 and resid 426 and name O)	6.09	0.34	0.34
	assign	(segid 3A4 and resid 424 and name O)	(segid 3A4 and resid 427 and name N)	7.00	0.29	0.29
	assign	(segid 3A4 and resid 425 and name C)	(segid 3A4 and resid 425 and name O)	1.24	0.01	0.01
	assign	(segid 3A4 and resid 425 and name C)	(segid 3A4 and resid 426 and name C)	3.32	0.08	0.07
60	assign	(segid 3A4 and resid 425 and name C)	(segid 3A4 and resid 426 and name CA)	2.44	0.01	0.02
	assign	(segid 3A4 and resid 425 and name C)	(segid 3A4 and resid 426 and name N)	1.33	0.01	0.01
	assign	(segid 3A4 and resid 425 and name C)	(segid 3A4 and resid 426 and name O)	3.65	0.19	0.20
	assign	(segid 3A4 and resid 425 and name C)	(segid 3A4 and resid 427 and name C)	6.36	0.16	0.16
65	assign	(segid 3A4 and resid 425 and name C)	(segid 3A4 and resid 427 and name CA)	5.42	0.05	0.05
	assign	(segid 3A4 and resid 425 and name C)	(segid 3A4 and resid 427 and name N)	4.24	0.06	0.05
	assign	(segid 3A4 and resid 425 and name C)	(segid 3A4 and resid 427 and name O)	6.56	0.28	0.28
	assign	(segid 3A4 and resid 425 and name C)	(segid 3A4 and resid 428 and name N)	7.22	0.25	0.24
	assign	(segid 3A4 and resid 425 and name C)	(segid 3A4 and resid 434 and name O)	5.97	0.95	0.95
	assign	(segid 3A4 and resid 425 and name C)	(segid 3A4 and resid 435 and name C)	5.82	0.67	0.67
70	assign	(segid 3A4 and resid 425 and name C)	(segid 3A4 and resid 435 and name CA)	5.48	0.67	0.67
	assign	(segid 3A4 and resid 425 and name C)	(segid 3A4 and resid 436 and name C)	6.50	0.71	0.72
	assign	(segid 3A4 and resid 425 and name C)	(segid 3A4 and resid 436 and name CA)	6.03	0.76	0.76
	assign	(segid 3A4 and resid 425 and name C)	(segid 3A4 and resid 436 and name N)	5.21	0.76	0.75
	assign	(segid 3A4 and resid 425 and name C)	(segid 3A4 and resid 425 and name C)	1.52	0.00	0.01
75	assign	(segid 3A4 and resid 425 and name CA)	(segid 3A4 and resid 425 and name O)	2.40	0.02	0.02
	assign	(segid 3A4 and resid 425 and name CA)	(segid 3A4 and resid 426 and name C)	4.58	0.05	0.05
	assign	(segid 3A4 and resid 425 and name CA)	(segid 3A4 and resid 426 and name CA)	3.81	0.02	0.01
	assign	(segid 3A4 and resid 425 and name CA)	(segid 3A4 and resid 426 and name N)	2.43	0.02	0.02
	assign	(segid 3A4 and resid 425 and name CA)	(segid 3A4 and resid 426 and name O)	4.63	0.15	0.15
80	assign	(segid 3A4 and resid 425 and name CA)	(segid 3A4 and resid 427 and name C)	7.59	0.19	0.18
	assign	(segid 3A4 and resid 425 and name CA)	(segid 3A4 and resid 427 and name CA)	6.66	0.14	0.14
	assign	(segid 3A4 and resid 425 and name CA)	(segid 3A4 and resid 427 and name N)	5.59	0.10	0.10
	assign	(segid 3A4 and resid 425 and name CA)	(segid 3A4 and resid 428 and name CA)	9.41	0.41	0.41

	assign (segid 3A4 and resid 425 and name CA)	(segid 3A4 and resid 429 and name CA)	12.35	0.65	0.64
	assign (segid 3A4 and resid 425 and name CA)	(segid 3A4 and resid 430 and name CA)	15.36	0.75	0.75
	assign (segid 3A4 and resid 425 and name CA)	(segid 3A4 and resid 431 and name CA)	16.52	1.66	1.66
	assign (segid 3A4 and resid 425 and name CA)	(segid 3A4 and resid 433 and name CA)	11.13	1.06	1.05
5	assign (segid 3A4 and resid 425 and name CA)	(segid 3A4 and resid 434 and name CA)	9.26	0.60	0.60
	assign (segid 3A4 and resid 425 and name CA)	(segid 3A4 and resid 435 and name C)	6.69	0.42	0.42
	assign (segid 3A4 and resid 425 and name CA)	(segid 3A4 and resid 435 and name CA)	6.39	0.39	0.39
	assign (segid 3A4 and resid 425 and name CA)	(segid 3A4 and resid 436 and name CA)	6.76	0.64	0.64
	assign (segid 3A4 and resid 425 and name CA)	(segid 3A4 and resid 436 and name N)	6.06	0.57	0.56
10	assign (segid 3A4 and resid 425 and name CA)	(segid 3A4 and resid 437 and name CA)	7.31	1.32	1.31
	assign (segid 3A4 and resid 425 and name CA)	(segid 3A4 and resid 438 and name CA)	8.03	1.43	1.43
	assign (segid 3A4 and resid 425 and name CA)	(segid 3A4 and resid 439 and name CA)	10.72	1.87	1.86
	assign (segid 3A4 and resid 425 and name CA)	(segid 3A4 and resid 440 and name CA)	13.29	1.64	1.65
	assign (segid 3A4 and resid 425 and name N)	(segid 3A4 and resid 425 and name C)	2.45	0.06	0.05
15	assign (segid 3A4 and resid 425 and name N)	(segid 3A4 and resid 425 and name O)	1.47	0.02	0.01
	assign (segid 3A4 and resid 425 and name N)	(segid 3A4 and resid 426 and name C)	2.94	0.14	0.13
	assign (segid 3A4 and resid 425 and name N)	(segid 3A4 and resid 426 and name CA)	5.70	0.09	0.09
	assign (segid 3A4 and resid 425 and name N)	(segid 3A4 and resid 426 and name N)	4.69	0.09	0.09
20	assign (segid 3A4 and resid 425 and name N)	(segid 3A4 and resid 426 and name O)	3.42	0.10	0.10
	assign (segid 3A4 and resid 425 and name N)	(segid 3A4 and resid 427 and name CA)	5.90	0.17	0.17
	assign (segid 3A4 and resid 425 and name N)	(segid 3A4 and resid 427 and name N)	7.81	0.06	0.07
	assign (segid 3A4 and resid 425 and name O)	(segid 3A4 and resid 426 and name C)	6.65	0.03	0.02
	assign (segid 3A4 and resid 425 and name O)	(segid 3A4 and resid 426 and name CA)	3.60	0.19	0.18
25	assign (segid 3A4 and resid 425 and name O)	(segid 3A4 and resid 426 and name N)	2.80	0.04	0.04
	assign (segid 3A4 and resid 425 and name O)	(segid 3A4 and resid 426 and name O)	2.27	0.03	0.02
	assign (segid 3A4 and resid 425 and name O)	(segid 3A4 and resid 427 and name C)	4.16	0.34	0.34
	assign (segid 3A4 and resid 425 and name O)	(segid 3A4 and resid 427 and name CA)	6.44	0.23	0.23
	assign (segid 3A4 and resid 425 and name O)	(segid 3A4 and resid 427 and name N)	5.37	0.19	0.19
30	assign (segid 3A4 and resid 425 and name O)	(segid 3A4 and resid 427 and name O)	4.19	0.15	0.16
	assign (segid 3A4 and resid 425 and name O)	(segid 3A4 and resid 428 and name N)	6.64	0.31	0.32
	assign (segid 3A4 and resid 425 and name O)	(segid 3A4 and resid 435 and name C)	7.39	0.25	0.25
	assign (segid 3A4 and resid 425 and name O)	(segid 3A4 and resid 435 and name CA)	5.41	1.40	1.39
	assign (segid 3A4 and resid 425 and name O)	(segid 3A4 and resid 436 and name CA)	5.18	1.31	1.31
35	assign (segid 3A4 and resid 425 and name O)	(segid 3A4 and resid 436 and name N)	5.57	1.47	1.46
	assign (segid 3A4 and resid 426 and name C)	(segid 3A4 and resid 426 and name O)	4.75	1.49	1.48
	assign (segid 3A4 and resid 426 and name C)	(segid 3A4 and resid 427 and name CA)	1.23	0.00	0.00
	assign (segid 3A4 and resid 426 and name C)	(segid 3A4 and resid 427 and name N)	3.14	0.13	0.12
	assign (segid 3A4 and resid 426 and name C)	(segid 3A4 and resid 427 and name O)	2.44	0.02	0.01
40	assign (segid 3A4 and resid 426 and name C)	(segid 3A4 and resid 427 and name O)	1.33	0.01	0.00
	assign (segid 3A4 and resid 426 and name C)	(segid 3A4 and resid 428 and name C)	3.42	0.24	0.24
	assign (segid 3A4 and resid 426 and name C)	(segid 3A4 and resid 428 and name N)	6.24	0.30	0.30
	assign (segid 3A4 and resid 426 and name C)	(segid 3A4 and resid 428 and name O)	5.15	0.17	0.18
45	assign (segid 3A4 and resid 426 and name C)	(segid 3A4 and resid 429 and name N)	4.04	0.16	0.16
	assign (segid 3A4 and resid 426 and name C)	(segid 3A4 and resid 434 and name C)	6.82	0.41	0.41
	assign (segid 3A4 and resid 426 and name C)	(segid 3A4 and resid 434 and name CA)	6.76	0.43	0.43
	assign (segid 3A4 and resid 426 and name C)	(segid 3A4 and resid 434 and name N)	5.11	0.33	0.34
	assign (segid 3A4 and resid 426 and name C)	(segid 3A4 and resid 435 and name C)	6.22	0.50	0.50
50	assign (segid 3A4 and resid 426 and name C)	(segid 3A4 and resid 435 and name CA)	6.10	0.74	0.74
	assign (segid 3A4 and resid 426 and name C)	(segid 3A4 and resid 435 and name N)	4.13	0.40	0.40
	assign (segid 3A4 and resid 426 and name C)	(segid 3A4 and resid 435 and name O)	5.41	0.46	0.46
	assign (segid 3A4 and resid 426 and name C)	(segid 3A4 and resid 436 and name CA)	5.05	0.36	0.36
	assign (segid 3A4 and resid 426 and name C)	(segid 3A4 and resid 436 and name N)	5.55	0.23	0.22
	assign (segid 3A4 and resid 426 and name C)	(segid 3A4 and resid 436 and name O)	6.43	0.42	0.41
55	assign (segid 3A4 and resid 426 and name C)	(segid 3A4 and resid 436 and name N)	5.83	0.70	0.69
	assign (segid 3A4 and resid 426 and name CA)	(segid 3A4 and resid 426 and name C)	4.94	0.66	0.66
	assign (segid 3A4 and resid 426 and name CA)	(segid 3A4 and resid 426 and name O)	1.53	0.01	0.00
	assign (segid 3A4 and resid 426 and name CA)	(segid 3A4 and resid 427 and name C)	2.40	0.01	0.00
60	assign (segid 3A4 and resid 426 and name CA)	(segid 3A4 and resid 427 and name N)	4.44	0.11	0.10
	assign (segid 3A4 and resid 426 and name CA)	(segid 3A4 and resid 427 and name O)	3.81	0.02	0.01
	assign (segid 3A4 and resid 426 and name CA)	(segid 3A4 and resid 428 and name C)	2.43	0.03	0.03
	assign (segid 3A4 and resid 426 and name CA)	(segid 3A4 and resid 428 and name N)	4.42	0.28	0.28
	assign (segid 3A4 and resid 426 and name CA)	(segid 3A4 and resid 428 and name O)	7.49	0.29	0.30
65	assign (segid 3A4 and resid 426 and name CA)	(segid 3A4 and resid 428 and name N)	6.41	0.14	0.13
	assign (segid 3A4 and resid 426 and name CA)	(segid 3A4 and resid 429 and name CA)	5.42	0.11	0.12
	assign (segid 3A4 and resid 426 and name CA)	(segid 3A4 and resid 430 and name CA)	9.10	0.57	0.56
	assign (segid 3A4 and resid 426 and name CA)	(segid 3A4 and resid 431 and name CA)	12.00	0.83	0.83
	assign (segid 3A4 and resid 426 and name CA)	(segid 3A4 and resid 433 and name CA)	13.23	1.90	1.91
	assign (segid 3A4 and resid 426 and name CA)	(segid 3A4 and resid 434 and name C)	7.99	1.54	1.53
70	assign (segid 3A4 and resid 426 and name CA)	(segid 3A4 and resid 434 and name CA)	5.40	1.00	1.00
	assign (segid 3A4 and resid 426 and name CA)	(segid 3A4 and resid 434 and name O)	6.62	1.15	1.14
	assign (segid 3A4 and resid 426 and name CA)	(segid 3A4 and resid 435 and name C)	4.48	1.06	1.06
	assign (segid 3A4 and resid 426 and name CA)	(segid 3A4 and resid 435 and name CA)	5.51	0.41	0.42
	assign (segid 3A4 and resid 426 and name CA)	(segid 3A4 and resid 435 and name N)	5.01	0.54	0.54
75	assign (segid 3A4 and resid 426 and name CA)	(segid 3A4 and resid 435 and name O)	5.66	0.79	0.80
	assign (segid 3A4 and resid 426 and name CA)	(segid 3A4 and resid 436 and name N)	6.58	0.47	0.47
	assign (segid 3A4 and resid 426 and name CA)	(segid 3A4 and resid 436 and name O)	6.03	0.53	0.53
	assign (segid 3A4 and resid 426 and name CA)	(segid 3A4 and resid 437 and name CA)	5.08	0.44	0.44
	assign (segid 3A4 and resid 426 and name CA)	(segid 3A4 and resid 438 and name CA)	8.09	0.82	0.82
80	assign (segid 3A4 and resid 426 and name CA)	(segid 3A4 and resid 439 and name CA)	9.59	1.08	1.07
	assign (segid 3A4 and resid 426 and name N)	(segid 3A4 and resid 440 and name CA)	12.84	1.29	1.28
	assign (segid 3A4 and resid 426 and name N)	(segid 3A4 and resid 426 and name C)	15.46	1.10	1.10
	assign (segid 3A4 and resid 426 and name N)	(segid 3A4 and resid 426 and name CA)	2.44	0.07	0.06
	assign (segid 3A4 and resid 426 and name N)	(segid 3A4 and resid 426 and name CA)	1.46	0.01	0.01

	assign (segid 3A4 and resid 426 and name N) (segid 3A4 and resid 426 and name O)	2.77	0.07	0.06
	assign (segid 3A4 and resid 426 and name N) (segid 3A4 and resid 427 and name C)	5.52	0.13	0.13
	assign (segid 3A4 and resid 426 and name N) (segid 3A4 and resid 427 and name CA)	4.78	0.12	0.12
	assign (segid 3A4 and resid 426 and name N) (segid 3A4 and resid 427 and name N)	3.55	0.10	0.09
5	assign (segid 3A4 and resid 426 and name N) (segid 3A4 and resid 427 and name O)	5.63	0.27	0.28
	assign (segid 3A4 and resid 426 and name N) (segid 3A4 and resid 428 and name CA)	7.37	0.27	0.27
	assign (segid 3A4 and resid 426 and name N) (segid 3A4 and resid 428 and name N)	6.36	0.23	0.23
	assign (segid 3A4 and resid 426 and name N) (segid 3A4 and resid 428 and name C)	6.25	0.67	0.67
	assign (segid 3A4 and resid 426 and name N) (segid 3A4 and resid 434 and name C)	5.44	0.76	0.76
	assign (segid 3A4 and resid 426 and name N) (segid 3A4 and resid 434 and name O)	5.81	0.38	0.38
10	assign (segid 3A4 and resid 426 and name N) (segid 3A4 and resid 435 and name C)	5.37	0.35	0.34
	assign (segid 3A4 and resid 426 and name N) (segid 3A4 and resid 435 and name CA)	6.27	0.50	0.50
	assign (segid 3A4 and resid 426 and name N) (segid 3A4 and resid 435 and name O)	6.91	0.40	0.40
	assign (segid 3A4 and resid 426 and name N) (segid 3A4 and resid 436 and name CA)	6.17	0.58	0.57
	assign (segid 3A4 and resid 426 and name N) (segid 3A4 and resid 436 and name N)	5.28	0.48	0.48
15	assign (segid 3A4 and resid 426 and name N) (segid 3A4 and resid 427 and name C)	3.31	0.26	0.27
	assign (segid 3A4 and resid 426 and name O) (segid 3A4 and resid 427 and name CA)	2.77	0.03	0.03
	assign (segid 3A4 and resid 426 and name O) (segid 3A4 and resid 427 and name N)	2.24	0.01	0.02
	assign (segid 3A4 and resid 426 and name O) (segid 3A4 and resid 427 and name O)	3.83	0.37	0.36
20	assign (segid 3A4 and resid 426 and name O) (segid 3A4 and resid 428 and name C)	6.14	0.45	0.45
	assign (segid 3A4 and resid 426 and name O) (segid 3A4 and resid 428 and name CA)	4.94	0.41	0.41
	assign (segid 3A4 and resid 426 and name O) (segid 3A4 and resid 428 and name N)	3.85	0.35	0.35
	assign (segid 3A4 and resid 426 and name O) (segid 3A4 and resid 428 and name O)	6.66	0.46	0.46
	assign (segid 3A4 and resid 426 and name O) (segid 3A4 and resid 429 and name N)	6.81	0.56	0.56
25	assign (segid 3A4 and resid 426 and name O) (segid 3A4 and resid 434 and name C)	5.64	0.48	0.48
	assign (segid 3A4 and resid 426 and name O) (segid 3A4 and resid 434 and name CA)	6.74	0.24	0.24
	assign (segid 3A4 and resid 426 and name O) (segid 3A4 and resid 434 and name N)	6.64	0.20	0.20
	assign (segid 3A4 and resid 426 and name O) (segid 3A4 and resid 434 and name O)	4.72	0.34	0.35
	assign (segid 3A4 and resid 426 and name O) (segid 3A4 and resid 435 and name C)	5.64	1.24	1.24
30	assign (segid 3A4 and resid 426 and name O) (segid 3A4 and resid 435 and name CA)	5.41	1.11	1.11
	assign (segid 3A4 and resid 426 and name O) (segid 3A4 and resid 435 and name N)	6.00	0.80	0.81
	assign (segid 3A4 and resid 426 and name O) (segid 3A4 and resid 436 and name CA)	5.87	1.32	1.32
	assign (segid 3A4 and resid 426 and name O) (segid 3A4 and resid 436 and name N)	5.06	1.38	1.38
	assign (segid 3A4 and resid 427 and name C) (segid 3A4 and resid 427 and name O)	1.23	0.00	0.00
35	assign (segid 3A4 and resid 427 and name C) (segid 3A4 and resid 428 and name C)	3.25	0.17	0.17
	assign (segid 3A4 and resid 427 and name C) (segid 3A4 and resid 428 and name CA)	2.43	0.02	0.02
	assign (segid 3A4 and resid 427 and name C) (segid 3A4 and resid 428 and name N)	1.33	0.01	0.00
	assign (segid 3A4 and resid 427 and name C) (segid 3A4 and resid 428 and name O)	3.88	0.37	0.38
	assign (segid 3A4 and resid 427 and name C) (segid 3A4 and resid 429 and name C)	6.02	0.43	0.42
40	assign (segid 3A4 and resid 427 and name C) (segid 3A4 and resid 429 and name CA)	5.02	0.29	0.29
	assign (segid 3A4 and resid 427 and name C) (segid 3A4 and resid 429 and name N)	3.78	0.28	0.28
	assign (segid 3A4 and resid 427 and name C) (segid 3A4 and resid 429 and name O)	6.30	0.68	0.69
	assign (segid 3A4 and resid 427 and name C) (segid 3A4 and resid 430 and name N)	6.84	0.48	0.48
	assign (segid 3A4 and resid 427 and name C) (segid 3A4 and resid 433 and name C)	5.94	0.52	0.52
45	assign (segid 3A4 and resid 427 and name C) (segid 3A4 and resid 433 and name CA)	5.73	0.68	0.68
	assign (segid 3A4 and resid 427 and name C) (segid 3A4 and resid 433 and name O)	7.02	0.47	0.47
	assign (segid 3A4 and resid 427 and name C) (segid 3A4 and resid 434 and name C)	5.34	0.52	0.52
	assign (segid 3A4 and resid 427 and name C) (segid 3A4 and resid 434 and name CA)	5.86	0.43	0.42
	assign (segid 3A4 and resid 427 and name C) (segid 3A4 and resid 434 and name N)	5.20	0.46	0.46
50	assign (segid 3A4 and resid 427 and name C) (segid 3A4 and resid 434 and name O)	4.36	0.58	0.58
	assign (segid 3A4 and resid 427 and name C) (segid 3A4 and resid 435 and name C)	6.73	0.69	0.70
	assign (segid 3A4 and resid 427 and name C) (segid 3A4 and resid 435 and name CA)	6.42	0.73	0.73
	assign (segid 3A4 and resid 427 and name C) (segid 3A4 and resid 435 and name N)	6.29	0.59	0.59
	assign (segid 3A4 and resid 427 and name C) (segid 3A4 and resid 436 and name N)	6.47	0.83	0.83
55	assign (segid 3A4 and resid 427 and name CA) (segid 3A4 and resid 427 and name C)	1.52	0.01	0.01
	assign (segid 3A4 and resid 427 and name CA) (segid 3A4 and resid 427 and name O)	2.39	0.01	0.01
	assign (segid 3A4 and resid 427 and name CA) (segid 3A4 and resid 428 and name C)	4.55	0.14	0.14
	assign (segid 3A4 and resid 427 and name CA) (segid 3A4 and resid 428 and name CA)	3.81	0.04	0.04
	assign (segid 3A4 and resid 427 and name CA) (segid 3A4 and resid 428 and name N)	2.44	0.05	0.04
60	assign (segid 3A4 and resid 427 and name CA) (segid 3A4 and resid 428 and name O)	4.98	0.44	0.43
	assign (segid 3A4 and resid 427 and name CA) (segid 3A4 and resid 429 and name C)	7.25	0.45	0.45
	assign (segid 3A4 and resid 427 and name CA) (segid 3A4 and resid 429 and name CA)	6.22	0.29	0.29
	assign (segid 3A4 and resid 427 and name CA) (segid 3A4 and resid 429 and name N)	5.12	0.29	0.29
	assign (segid 3A4 and resid 427 and name CA) (segid 3A4 and resid 430 and name CA)	9.24	0.52	0.52
65	assign (segid 3A4 and resid 427 and name CA) (segid 3A4 and resid 431 and name CA)	10.31	1.66	1.67
	assign (segid 3A4 and resid 427 and name CA) (segid 3A4 and resid 433 and name C)	5.94	0.40	0.41
	assign (segid 3A4 and resid 427 and name CA) (segid 3A4 and resid 433 and name CA)	6.00	0.61	0.61
	assign (segid 3A4 and resid 427 and name CA) (segid 3A4 and resid 433 and name O)	6.90	0.40	0.40
	assign (segid 3A4 and resid 427 and name CA) (segid 3A4 and resid 434 and name C)	4.77	0.34	0.34
70	assign (segid 3A4 and resid 427 and name CA) (segid 3A4 and resid 434 and name CA)	5.52	0.22	0.22
	assign (segid 3A4 and resid 427 and name CA) (segid 3A4 and resid 434 and name N)	5.13	0.25	0.24
	assign (segid 3A4 and resid 427 and name CA) (segid 3A4 and resid 434 and name O)	3.78	0.33	0.33
	assign (segid 3A4 and resid 427 and name CA) (segid 3A4 and resid 435 and name C)	5.79	0.44	0.45
	assign (segid 3A4 and resid 427 and name CA) (segid 3A4 and resid 435 and name CA)	5.50	0.66	0.67
75	assign (segid 3A4 and resid 427 and name CA) (segid 3A4 and resid 435 and name N)	5.54	0.51	0.51
	assign (segid 3A4 and resid 427 and name CA) (segid 3A4 and resid 435 and name O)	6.60	0.26	0.26
	assign (segid 3A4 and resid 427 and name CA) (segid 3A4 and resid 436 and name CA)	6.29	0.43	0.43
	assign (segid 3A4 and resid 427 and name CA) (segid 3A4 and resid 436 and name N)	5.52	0.58	0.59
	assign (segid 3A4 and resid 427 and name CA) (segid 3A4 and resid 437 and name CA)	9.35	0.48	0.49
80	assign (segid 3A4 and resid 427 and name CA) (segid 3A4 and resid 438 and name CA)	11.44	1.05	1.06
	assign (segid 3A4 and resid 427 and name CA) (segid 3A4 and resid 439 and name CA)	14.91	1.07	1.08
	assign (segid 3A4 and resid 427 and name N) (segid 3A4 and resid 427 and name C)	2.38	0.06	0.05
	assign (segid 3A4 and resid 427 and name N) (segid 3A4 and resid 427 and name CA)	1.46	0.01	0.01

	assign (segid 3A4 and resid 427 and name N)	(segid 3A4 and resid 427 and name O)	2.69	0.13	0.13
	assign (segid 3A4 and resid 427 and name N)	(segid 3A4 and resid 428 and name C)	5.59	0.18	0.17
	assign (segid 3A4 and resid 427 and name N)	(segid 3A4 and resid 428 and name CA)	4.70	0.09	0.10
	assign (segid 3A4 and resid 427 and name N)	(segid 3A4 and resid 428 and name N)	3.50	0.08	0.07
5	assign (segid 3A4 and resid 427 and name N)	(segid 3A4 and resid 428 and name O)	6.14	0.43	0.43
	assign (segid 3A4 and resid 427 and name N)	(segid 3A4 and resid 429 and name CA)	7.17	0.35	0.34
	assign (segid 3A4 and resid 427 and name N)	(segid 3A4 and resid 429 and name N)	6.03	0.31	0.30
	assign (segid 3A4 and resid 427 and name N)	(segid 3A4 and resid 434 and name C)	4.57	0.58	0.59
	assign (segid 3A4 and resid 427 and name N)	(segid 3A4 and resid 434 and name CA)	5.54	0.77	0.77
	assign (segid 3A4 and resid 427 and name N)	(segid 3A4 and resid 434 and name N)	5.29	0.92	0.92
10	assign (segid 3A4 and resid 427 and name N)	(segid 3A4 and resid 434 and name O)	3.54	0.58	0.58
	assign (segid 3A4 and resid 427 and name N)	(segid 3A4 and resid 435 and name C)	5.36	0.19	0.20
	assign (segid 3A4 and resid 427 and name N)	(segid 3A4 and resid 435 and name CA)	4.98	0.27	0.27
	assign (segid 3A4 and resid 427 and name N)	(segid 3A4 and resid 435 and name N)	5.22	0.42	0.42
	assign (segid 3A4 and resid 427 and name N)	(segid 3A4 and resid 435 and name O)	6.28	0.36	0.36
15	assign (segid 3A4 and resid 427 and name N)	(segid 3A4 and resid 436 and name C)	7.08	0.37	0.37
	assign (segid 3A4 and resid 427 and name N)	(segid 3A4 and resid 436 and name CA)	5.94	0.30	0.31
	assign (segid 3A4 and resid 427 and name N)	(segid 3A4 and resid 436 and name N)	5.05	0.31	0.32
	assign (segid 3A4 and resid 427 and name N)	(segid 3A4 and resid 428 and name C)	3.41	0.31	0.31
	assign (segid 3A4 and resid 427 and name O)	(segid 3A4 and resid 428 and name CA)	2.73	0.05	0.05
20	assign (segid 3A4 and resid 427 and name O)	(segid 3A4 and resid 428 and name N)	2.24	0.02	0.02
	assign (segid 3A4 and resid 427 and name O)	(segid 3A4 and resid 428 and name O)	4.25	0.46	0.46
	assign (segid 3A4 and resid 427 and name O)	(segid 3A4 and resid 429 and name C)	5.72	0.69	0.68
	assign (segid 3A4 and resid 427 and name O)	(segid 3A4 and resid 429 and name CA)	4.80	0.49	0.50
	assign (segid 3A4 and resid 427 and name O)	(segid 3A4 and resid 429 and name N)	3.59	0.42	0.43
25	assign (segid 3A4 and resid 427 and name O)	(segid 3A4 and resid 429 and name O)	5.85	0.94	0.94
	assign (segid 3A4 and resid 427 and name O)	(segid 3A4 and resid 433 and name C)	5.86	1.11	1.11
	assign (segid 3A4 and resid 427 and name O)	(segid 3A4 and resid 433 and name CA)	5.55	1.20	1.20
	assign (segid 3A4 and resid 427 and name O)	(segid 3A4 and resid 434 and name C)	5.52	0.60	0.60
	assign (segid 3A4 and resid 427 and name O)	(segid 3A4 and resid 434 and name CA)	5.92	0.83	0.84
30	assign (segid 3A4 and resid 427 and name O)	(segid 3A4 and resid 434 and name N)	5.14	1.00	1.00
	assign (segid 3A4 and resid 427 and name O)	(segid 3A4 and resid 434 and name O)	4.58	0.52	0.51
	assign (segid 3A4 and resid 427 and name O)	(segid 3A4 and resid 435 and name CA)	6.72	0.49	0.50
	assign (segid 3A4 and resid 427 and name O)	(segid 3A4 and resid 435 and name N)	6.52	0.52	0.53
	assign (segid 3A4 and resid 427 and name O)	(segid 3A4 and resid 436 and name N)	6.92	0.63	0.63
35	assign (segid 3A4 and resid 428 and name C)	(segid 3A4 and resid 428 and name O)	1.23	0.01	0.01
	assign (segid 3A4 and resid 428 and name C)	(segid 3A4 and resid 429 and name C)	3.36	0.18	0.18
	assign (segid 3A4 and resid 428 and name C)	(segid 3A4 and resid 429 and name CA)	2.44	0.02	0.01
	assign (segid 3A4 and resid 428 and name C)	(segid 3A4 and resid 429 and name N)	1.32	0.01	0.01
	assign (segid 3A4 and resid 428 and name C)	(segid 3A4 and resid 429 and name O)	3.99	0.13	0.13
40	assign (segid 3A4 and resid 428 and name C)	(segid 3A4 and resid 430 and name C)	5.98	0.82	0.81
	assign (segid 3A4 and resid 428 and name C)	(segid 3A4 and resid 430 and name CA)	5.27	0.54	0.53
	assign (segid 3A4 and resid 428 and name C)	(segid 3A4 and resid 430 and name N)	3.98	0.51	0.52
	assign (segid 3A4 and resid 428 and name C)	(segid 3A4 and resid 430 and name O)	6.57	1.01	1.01
	assign (segid 3A4 and resid 428 and name C)	(segid 3A4 and resid 431 and name N)	6.23	1.05	1.05
45	assign (segid 3A4 and resid 428 and name C)	(segid 3A4 and resid 433 and name C)	6.38	1.07	1.07
	assign (segid 3A4 and resid 428 and name C)	(segid 3A4 and resid 433 and name CA)	5.69	0.92	0.92
	assign (segid 3A4 and resid 428 and name C)	(segid 3A4 and resid 433 and name N)	6.28	0.72	0.71
	assign (segid 3A4 and resid 428 and name C)	(segid 3A4 and resid 434 and name N)	6.00	1.26	1.27
	assign (segid 3A4 and resid 428 and name C)	(segid 3A4 and resid 428 and name O)	1.53	0.01	0.01
50	assign (segid 3A4 and resid 428 and name CA)	(segid 3A4 and resid 428 and name C)	2.40	0.02	0.02
	assign (segid 3A4 and resid 428 and name CA)	(segid 3A4 and resid 429 and name C)	4.66	0.10	0.09
	assign (segid 3A4 and resid 428 and name CA)	(segid 3A4 and resid 429 and name CA)	3.81	0.03	0.02
	assign (segid 3A4 and resid 428 and name CA)	(segid 3A4 and resid 429 and name N)	2.43	0.03	0.03
	assign (segid 3A4 and resid 428 and name CA)	(segid 3A4 and resid 429 and name O)	5.08	0.28	0.28
55	assign (segid 3A4 and resid 428 and name CA)	(segid 3A4 and resid 430 and name CA)	6.50	0.52	0.51
	assign (segid 3A4 and resid 428 and name CA)	(segid 3A4 and resid 430 and name N)	5.32	0.51	0.50
	assign (segid 3A4 and resid 428 and name CA)	(segid 3A4 and resid 431 and name CA)	8.40	1.37	1.37
	assign (segid 3A4 and resid 428 and name CA)	(segid 3A4 and resid 433 and name CA)	6.22	1.03	1.03
	assign (segid 3A4 and resid 428 and name CA)	(segid 3A4 and resid 434 and name CA)	7.01	1.25	1.24
60	assign (segid 3A4 and resid 428 and name CA)	(segid 3A4 and resid 434 and name N)	6.15	1.19	1.19
	assign (segid 3A4 and resid 428 and name CA)	(segid 3A4 and resid 434 and name O)	5.97	1.30	1.31
	assign (segid 3A4 and resid 428 and name CA)	(segid 3A4 and resid 435 and name CA)	8.19	1.28	1.28
	assign (segid 3A4 and resid 428 and name CA)	(segid 3A4 and resid 436 and name CA)	8.72	1.54	1.53
	assign (segid 3A4 and resid 428 and name CA)	(segid 3A4 and resid 437 and name CA)	11.86	1.21	1.22
65	assign (segid 3A4 and resid 428 and name CA)	(segid 3A4 and resid 438 and name CA)	14.26	1.51	1.51
	assign (segid 3A4 and resid 428 and name CA)	(segid 3A4 and resid 428 and name C)	2.46	0.05	0.05
	assign (segid 3A4 and resid 428 and name N)	(segid 3A4 and resid 428 and name CA)	1.47	0.01	0.01
	assign (segid 3A4 and resid 428 and name N)	(segid 3A4 and resid 428 and name O)	3.01	0.23	0.23
	assign (segid 3A4 and resid 428 and name N)	(segid 3A4 and resid 429 and name C)	5.61	0.12	0.11
70	assign (segid 3A4 and resid 428 and name N)	(segid 3A4 and resid 429 and name CA)	4.62	0.12	0.13
	assign (segid 3A4 and resid 428 and name N)	(segid 3A4 and resid 429 and name N)	3.34	0.15	0.15
	assign (segid 3A4 and resid 428 and name N)	(segid 3A4 and resid 429 and name O)	6.02	0.34	0.35
	assign (segid 3A4 and resid 428 and name N)	(segid 3A4 and resid 430 and name N)	6.29	0.45	0.44
	assign (segid 3A4 and resid 428 and name N)	(segid 3A4 and resid 433 and name C)	6.32	0.73	0.73
75	assign (segid 3A4 and resid 428 and name N)	(segid 3A4 and resid 433 and name CA)	6.04	0.68	0.68
	assign (segid 3A4 and resid 428 and name N)	(segid 3A4 and resid 433 and name N)	6.98	0.51	0.51
	assign (segid 3A4 and resid 428 and name N)	(segid 3A4 and resid 434 and name C)	5.91	1.22	1.21
	assign (segid 3A4 and resid 428 and name N)	(segid 3A4 and resid 434 and name CA)	6.32	1.04	1.04
	assign (segid 3A4 and resid 428 and name N)	(segid 3A4 and resid 434 and name N)	5.63	0.92	0.92
80	assign (segid 3A4 and resid 428 and name N)	(segid 3A4 and resid 434 and name O)	1.97	1.29	1.29
	assign (segid 3A4 and resid 428 and name O)	(segid 3A4 and resid 429 and name C)	3.60	0.40	0.39
	assign (segid 3A4 and resid 428 and name O)	(segid 3A4 and resid 429 and name CA)	2.78	0.04	0.04

	assign (segid 3A4 and resid 428 and name O)	(segid 3A4 and resid 429 and name N)	2.24	0.02	0.02
	assign (segid 3A4 and resid 428 and name O)	(segid 3A4 and resid 429 and name O)	4.38	0.32	0.31
	assign (segid 3A4 and resid 428 and name O)	(segid 3A4 and resid 430 and name C)	5.77	1.13	1.13
	assign (segid 3A4 and resid 428 and name O)	(segid 3A4 and resid 430 and name CA)	5.18	0.85	0.86
5	assign (segid 3A4 and resid 428 and name O)	(segid 3A4 and resid 430 and name N)	3.93	0.74	0.75
	assign (segid 3A4 and resid 428 and name O)	(segid 3A4 and resid 431 and name N)	5.95	1.29	1.29
	assign (segid 3A4 and resid 428 and name O)	(segid 3A4 and resid 433 and name CA)	5.59	1.38	1.38
	assign (segid 3A4 and resid 428 and name O)	(segid 3A4 and resid 433 and name N)	6.10	1.09	1.10
	assign (segid 3A4 and resid 428 and name O)	(segid 3A4 and resid 433 and name N)	1.23	0.01	0.00
10	assign (segid 3A4 and resid 429 and name C)	(segid 3A4 and resid 429 and name O)	3.35	0.14	0.13
	assign (segid 3A4 and resid 429 and name C)	(segid 3A4 and resid 430 and name CA)	2.44	0.03	0.03
	assign (segid 3A4 and resid 429 and name C)	(segid 3A4 and resid 430 and name N)	1.33	0.01	0.01
	assign (segid 3A4 and resid 429 and name C)	(segid 3A4 and resid 430 and name O)	4.11	0.28	0.27
	assign (segid 3A4 and resid 429 and name C)	(segid 3A4 and resid 431 and name C)	5.20	0.44	0.43
15	assign (segid 3A4 and resid 429 and name C)	(segid 3A4 and resid 431 and name CA)	5.06	0.49	0.49
	assign (segid 3A4 and resid 429 and name C)	(segid 3A4 and resid 431 and name N)	3.79	0.52	0.53
	assign (segid 3A4 and resid 429 and name C)	(segid 3A4 and resid 431 and name O)	5.69	0.78	0.79
	assign (segid 3A4 and resid 429 and name C)	(segid 3A4 and resid 433 and name CA)	5.83	0.79	0.80
	assign (segid 3A4 and resid 429 and name C)	(segid 3A4 and resid 433 and name N)	5.77	0.63	0.64
20	assign (segid 3A4 and resid 429 and name CA)	(segid 3A4 and resid 429 and name O)	1.52	0.01	0.01
	assign (segid 3A4 and resid 429 and name CA)	(segid 3A4 and resid 429 and name O)	2.40	0.01	0.01
	assign (segid 3A4 and resid 429 and name CA)	(segid 3A4 and resid 430 and name C)	4.57	0.08	0.09
	assign (segid 3A4 and resid 429 and name CA)	(segid 3A4 and resid 430 and name CA)	3.81	0.04	0.04
	assign (segid 3A4 and resid 429 and name CA)	(segid 3A4 and resid 430 and name N)	2.42	0.03	0.04
25	assign (segid 3A4 and resid 429 and name CA)	(segid 3A4 and resid 430 and name O)	5.23	0.45	0.44
	assign (segid 3A4 and resid 429 and name CA)	(segid 3A4 and resid 431 and name C)	5.98	0.42	0.41
	assign (segid 3A4 and resid 429 and name CA)	(segid 3A4 and resid 431 and name CA)	6.01	0.55	0.54
	assign (segid 3A4 and resid 429 and name CA)	(segid 3A4 and resid 431 and name N)	4.89	0.59	0.59
	assign (segid 3A4 and resid 429 and name CA)	(segid 3A4 and resid 431 and name O)	6.42	0.74	0.74
30	assign (segid 3A4 and resid 429 and name CA)	(segid 3A4 and resid 433 and name CA)	5.69	0.83	0.82
	assign (segid 3A4 and resid 429 and name CA)	(segid 3A4 and resid 433 and name N)	5.89	0.64	0.65
	assign (segid 3A4 and resid 429 and name CA)	(segid 3A4 and resid 434 and name CA)	7.75	0.95	0.95
	assign (segid 3A4 and resid 429 and name CA)	(segid 3A4 and resid 435 and name CA)	10.11	0.75	0.74
	assign (segid 3A4 and resid 429 and name CA)	(segid 3A4 and resid 436 and name CA)	11.07	0.86	0.86
35	assign (segid 3A4 and resid 429 and name CA)	(segid 3A4 and resid 437 and name CA)	14.26	0.69	0.69
	assign (segid 3A4 and resid 429 and name CA)	(segid 3A4 and resid 438 and name CA)	16.51	0.86	0.86
	assign (segid 3A4 and resid 429 and name N)	(segid 3A4 and resid 429 and name C)	2.48	0.06	0.06
	assign (segid 3A4 and resid 429 and name N)	(segid 3A4 and resid 429 and name O)	1.46	0.02	0.01
	assign (segid 3A4 and resid 429 and name N)	(segid 3A4 and resid 429 and name O)	3.05	0.29	0.29
40	assign (segid 3A4 and resid 429 and name N)	(segid 3A4 and resid 430 and name C)	5.48	0.36	0.36
	assign (segid 3A4 and resid 429 and name N)	(segid 3A4 and resid 430 and name CA)	4.69	0.19	0.18
	assign (segid 3A4 and resid 429 and name N)	(segid 3A4 and resid 430 and name N)	3.37	0.23	0.23
	assign (segid 3A4 and resid 429 and name N)	(segid 3A4 and resid 430 and name O)	6.11	0.49	0.49
	assign (segid 3A4 and resid 429 and name N)	(segid 3A4 and resid 431 and name N)	5.80	0.76	0.75
45	assign (segid 3A4 and resid 429 and name N)	(segid 3A4 and resid 433 and name CA)	5.65	0.83	0.84
	assign (segid 3A4 and resid 429 and name N)	(segid 3A4 and resid 433 and name N)	6.13	0.70	0.70
	assign (segid 3A4 and resid 429 and name O)	(segid 3A4 and resid 430 and name C)	3.66	0.27	0.27
	assign (segid 3A4 and resid 429 and name O)	(segid 3A4 and resid 430 and name CA)	2.77	0.03	0.03
50	assign (segid 3A4 and resid 429 and name O)	(segid 3A4 and resid 430 and name N)	2.25	0.01	0.00
	assign (segid 3A4 and resid 429 and name O)	(segid 3A4 and resid 430 and name O)	4.43	0.21	0.20
	assign (segid 3A4 and resid 429 and name O)	(segid 3A4 and resid 431 and name C)	5.38	0.77	0.76
	assign (segid 3A4 and resid 429 and name O)	(segid 3A4 and resid 431 and name CA)	5.30	0.66	0.67
	assign (segid 3A4 and resid 429 and name O)	(segid 3A4 and resid 431 and name N)	4.07	0.62	0.62
	assign (segid 3A4 and resid 429 and name O)	(segid 3A4 and resid 431 and name O)	5.86	1.14	1.13
55	assign (segid 3A4 and resid 429 and name O)	(segid 3A4 and resid 433 and name CA)	5.87	0.94	0.95
	assign (segid 3A4 and resid 429 and name O)	(segid 3A4 and resid 433 and name N)	5.80	0.84	0.84
	assign (segid 3A4 and resid 42 and name C)	(segid 3A4 and resid 42 and name CB)	2.52	0.03	0.03
	assign (segid 3A4 and resid 42 and name C)	(segid 3A4 and resid 42 and name O)	1.23	0.01	0.01
	assign (segid 3A4 and resid 42 and name CA)	(segid 3A4 and resid 319 and name CA)	16.72	0.72	0.73
60	assign (segid 3A4 and resid 42 and name CA)	(segid 3A4 and resid 319 and name CB)	16.18	0.77	0.78
	assign (segid 3A4 and resid 42 and name CA)	(segid 3A4 and resid 322 and name CA)	10.25	1.33	1.33
	assign (segid 3A4 and resid 42 and name CA)	(segid 3A4 and resid 323 and name CA)	8.54	0.88	0.89
	assign (segid 3A4 and resid 42 and name CA)	(segid 3A4 and resid 323 and name CB)	7.09	0.86	0.87
	assign (segid 3A4 and resid 42 and name CA)	(segid 3A4 and resid 324 and name CA)	10.19	0.56	0.57
65	assign (segid 3A4 and resid 42 and name CA)	(segid 3A4 and resid 324 and name CB)	11.64	0.56	0.56
	assign (segid 3A4 and resid 42 and name CA)	(segid 3A4 and resid 325 and name CA)	9.63	0.46	0.46
	assign (segid 3A4 and resid 42 and name CA)	(segid 3A4 and resid 325 and name CB)	9.71	0.39	0.40
	assign (segid 3A4 and resid 42 and name CA)	(segid 3A4 and resid 326 and name CA)	12.04	0.50	0.50
	assign (segid 3A4 and resid 42 and name CA)	(segid 3A4 and resid 326 and name CB)	11.99	0.55	0.55
70	assign (segid 3A4 and resid 42 and name CA)	(segid 3A4 and resid 327 and name CA)	13.07	0.50	0.49
	assign (segid 3A4 and resid 42 and name CA)	(segid 3A4 and resid 327 and name CB)	13.22	0.53	0.54
	assign (segid 3A4 and resid 42 and name CA)	(segid 3A4 and resid 328 and name CA)	13.06	0.49	0.49
	assign (segid 3A4 and resid 42 and name CA)	(segid 3A4 and resid 328 and name CB)	14.38	0.53	0.53
	assign (segid 3A4 and resid 42 and name CA)	(segid 3A4 and resid 329 and name CA)	10.33	0.67	0.67
75	assign (segid 3A4 and resid 42 and name CA)	(segid 3A4 and resid 329 and name CB)	9.01	0.67	0.67
	assign (segid 3A4 and resid 42 and name CA)	(segid 3A4 and resid 330 and name CA)	10.56	0.63	0.64
	assign (segid 3A4 and resid 42 and name CA)	(segid 3A4 and resid 330 and name CB)	11.83	0.65	0.65
	assign (segid 3A4 and resid 42 and name CA)	(segid 3A4 and resid 331 and name CA)	8.06	0.54	0.54
	assign (segid 3A4 and resid 42 and name CA)	(segid 3A4 and resid 331 and name CB)	7.06	0.49	0.50
80	assign (segid 3A4 and resid 42 and name CA)	(segid 3A4 and resid 332 and name CA)	10.32	0.66	0.66
	assign (segid 3A4 and resid 42 and name CA)	(segid 3A4 and resid 332 and name CB)	13.34	0.61	0.65
	assign (segid 3A4 and resid 42 and name CA)	(segid 3A4 and resid 333 and name CA)	12.65	0.48	0.48
	assign (segid 3A4 and resid 42 and name CA)	(segid 3A4 and resid 335 and name CA)	12.92	0.55	0.54

	assign (segid 3A4 and resid 42 and name CA)	(segid 3A4 and resid 336 and name CB)	14.35	0.56	0.55
	assign (segid 3A4 and resid 42 and name CA)	(segid 3A4 and resid 337 and name CA)	11.37	0.37	0.37
	assign (segid 3A4 and resid 42 and name CA)	(segid 3A4 and resid 337 and name CB)	9.92	0.37	0.37
	assign (segid 3A4 and resid 42 and name CA)	(segid 3A4 and resid 338 and name CA)	13.96	0.37	0.36
	assign (segid 3A4 and resid 42 and name CA)	(segid 3A4 and resid 338 and name CB)	15.26	0.41	0.40
5	assign (segid 3A4 and resid 42 and name CA)	(segid 3A4 and resid 339 and name CA)	14.03	0.38	0.38
	assign (segid 3A4 and resid 42 and name CA)	(segid 3A4 and resid 339 and name CB)	15.14	0.37	0.36
	assign (segid 3A4 and resid 42 and name CA)	(segid 3A4 and resid 340 and name CA)	14.39	0.59	0.58
	assign (segid 3A4 and resid 42 and name CA)	(segid 3A4 and resid 341 and name CA)	12.80	0.52	0.52
	assign (segid 3A4 and resid 42 and name CA)	(segid 3A4 and resid 341 and name CB)	12.34	0.48	0.48
10	assign (segid 3A4 and resid 42 and name CA)	(segid 3A4 and resid 342 and name CA)	11.64	0.62	0.63
	assign (segid 3A4 and resid 42 and name CA)	(segid 3A4 and resid 343 and name CA)	8.80	0.53	0.53
	assign (segid 3A4 and resid 42 and name CA)	(segid 3A4 and resid 343 and name CB)	7.42	0.56	0.57
	assign (segid 3A4 and resid 42 and name CA)	(segid 3A4 and resid 344 and name CA)	9.70	0.57	0.56
	assign (segid 3A4 and resid 42 and name CA)	(segid 3A4 and resid 344 and name CB)	11.15	0.55	0.55
15	assign (segid 3A4 and resid 42 and name CA)	(segid 3A4 and resid 345 and name CA)	7.94	0.65	0.65
	assign (segid 3A4 and resid 42 and name CA)	(segid 3A4 and resid 345 and name CB)	6.92	0.80	0.80
	assign (segid 3A4 and resid 42 and name CA)	(segid 3A4 and resid 346 and name CA)	11.08	0.57	0.57
	assign (segid 3A4 and resid 42 and name CA)	(segid 3A4 and resid 346 and name CB)	11.90	0.41	0.40
	assign (segid 3A4 and resid 42 and name CA)	(segid 3A4 and resid 347 and name CA)	11.63	0.65	0.66
20	assign (segid 3A4 and resid 42 and name CA)	(segid 3A4 and resid 347 and name CB)	12.01	0.71	0.72
	assign (segid 3A4 and resid 42 and name CA)	(segid 3A4 and resid 348 and name CA)	15.09	0.64	0.63
	assign (segid 3A4 and resid 42 and name CA)	(segid 3A4 and resid 349 and name CA)	14.18	0.39	0.39
	assign (segid 3A4 and resid 42 and name CA)	(segid 3A4 and resid 349 and name CB)	13.56	0.38	0.39
	assign (segid 3A4 and resid 42 and name CA)	(segid 3A4 and resid 350 and name CA)	12.30	0.40	0.39
25	assign (segid 3A4 and resid 42 and name CA)	(segid 3A4 and resid 350 and name CB)	11.17	0.46	0.47
	assign (segid 3A4 and resid 42 and name CA)	(segid 3A4 and resid 351 and name CA)	15.43	0.46	0.46
	assign (segid 3A4 and resid 42 and name CA)	(segid 3A4 and resid 352 and name CA)	17.59	0.43	0.43
	assign (segid 3A4 and resid 42 and name CA)	(segid 3A4 and resid 352 and name CB)	18.12	0.47	0.48
	assign (segid 3A4 and resid 42 and name CA)	(segid 3A4 and resid 353 and name CA)	16.16	0.47	0.48
30	assign (segid 3A4 and resid 42 and name CA)	(segid 3A4 and resid 353 and name CB)	14.84	0.57	0.56
	assign (segid 3A4 and resid 42 and name CA)	(segid 3A4 and resid 355 and name CA)	17.13	0.99	0.99
	assign (segid 3A4 and resid 42 and name CA)	(segid 3A4 and resid 356 and name CA)	17.23	0.78	0.78
	assign (segid 3A4 and resid 42 and name CA)	(segid 3A4 and resid 356 and name CB)	15.91	0.76	0.77
	assign (segid 3A4 and resid 42 and name CA)	(segid 3A4 and resid 381 and name CA)	14.94	0.61	0.62
35	assign (segid 3A4 and resid 42 and name CA)	(segid 3A4 and resid 382 and name CA)	12.38	0.45	0.45
	assign (segid 3A4 and resid 42 and name CA)	(segid 3A4 and resid 382 and name CB)	10.99	0.46	0.46
	assign (segid 3A4 and resid 42 and name CA)	(segid 3A4 and resid 383 and name CA)	15.07	0.36	0.36
	assign (segid 3A4 and resid 42 and name CA)	(segid 3A4 and resid 384 and name CA)	14.86	0.32	0.31
	assign (segid 3A4 and resid 42 and name CA)	(segid 3A4 and resid 384 and name CB)	15.75	0.29	0.29
40	assign (segid 3A4 and resid 42 and name CA)	(segid 3A4 and resid 385 and name CA)	11.15	0.34	0.35
	assign (segid 3A4 and resid 42 and name CA)	(segid 3A4 and resid 386 and name CA)	9.38	0.26	0.26
	assign (segid 3A4 and resid 42 and name CA)	(segid 3A4 and resid 387 and name CA)	9.22	0.83	0.84
	assign (segid 3A4 and resid 42 and name CA)	(segid 3A4 and resid 388 and name CA)	11.61	0.99	0.99
	assign (segid 3A4 and resid 42 and name CA)	(segid 3A4 and resid 388 and name CB)	11.69	1.16	1.15
45	assign (segid 3A4 and resid 42 and name CA)	(segid 3A4 and resid 389 and name CA)	12.04	0.57	0.58
	assign (segid 3A4 and resid 42 and name CA)	(segid 3A4 and resid 389 and name CB)	11.38	0.53	0.52
	assign (segid 3A4 and resid 42 and name CA)	(segid 3A4 and resid 390 and name CA)	12.95	0.52	0.51
	assign (segid 3A4 and resid 42 and name CA)	(segid 3A4 and resid 390 and name CB)	13.11	0.55	0.55
	assign (segid 3A4 and resid 42 and name CA)	(segid 3A4 and resid 391 and name CA)	16.18	0.50	0.51
50	assign (segid 3A4 and resid 42 and name CA)	(segid 3A4 and resid 391 and name CB)	16.69	0.47	0.47
	assign (segid 3A4 and resid 42 and name CA)	(segid 3A4 and resid 392 and name CA)	19.05	0.54	0.55
	assign (segid 3A4 and resid 42 and name CA)	(segid 3A4 and resid 42 and name C)	1.52	0.00	0.01
	assign (segid 3A4 and resid 42 and name CA)	(segid 3A4 and resid 42 and name CB)	1.53	0.02	0.01
	assign (segid 3A4 and resid 42 and name CA)	(segid 3A4 and resid 42 and name O)	2.39	0.01	0.01
55	assign (segid 3A4 and resid 42 and name CA)	(segid 3A4 and resid 68 and name CA)	16.61	1.49	1.49
	assign (segid 3A4 and resid 42 and name CA)	(segid 3A4 and resid 69 and name CA)	16.91	1.41	1.42
	assign (segid 3A4 and resid 42 and name CA)	(segid 3A4 and resid 70 and name CA)	16.91	1.48	1.49
	assign (segid 3A4 and resid 42 and name CA)	(segid 3A4 and resid 71 and name CA)	15.12	1.82	1.82
60	assign (segid 3A4 and resid 42 and name CA)	(segid 3A4 and resid 72 and name CA)	15.78	1.02	1.02
	assign (segid 3A4 and resid 42 and name CA)	(segid 3A4 and resid 75 and name CB)	16.65	1.42	1.43
	assign (segid 3A4 and resid 42 and name CB)	(segid 3A4 and resid 317 and name CA)	17.62	0.67	0.68
	assign (segid 3A4 and resid 42 and name CB)	(segid 3A4 and resid 319 and name CA)	15.84	0.62	0.63
	assign (segid 3A4 and resid 42 and name CB)	(segid 3A4 and resid 319 and name CB)	15.41	0.66	0.65
	assign (segid 3A4 and resid 42 and name CB)	(segid 3A4 and resid 322 and name CA)	9.24	1.28	1.28
65	assign (segid 3A4 and resid 42 and name CB)	(segid 3A4 and resid 323 and name CA)	7.84	0.78	0.79
	assign (segid 3A4 and resid 42 and name CB)	(segid 3A4 and resid 323 and name CB)	6.46	0.76	0.77
	assign (segid 3A4 and resid 42 and name CB)	(segid 3A4 and resid 324 and name CA)	9.66	0.42	0.42
	assign (segid 3A4 and resid 42 and name CB)	(segid 3A4 and resid 324 and name CB)	11.15	0.41	0.40
	assign (segid 3A4 and resid 42 and name CB)	(segid 3A4 and resid 325 and name CA)	9.42	0.28	0.28
70	assign (segid 3A4 and resid 42 and name CB)	(segid 3A4 and resid 325 and name CB)	9.45	0.24	0.23
	assign (segid 3A4 and resid 42 and name CB)	(segid 3A4 and resid 326 and name CA)	12.21	0.33	0.33
	assign (segid 3A4 and resid 42 and name CB)	(segid 3A4 and resid 326 and name CB)	12.31	0.39	0.39
	assign (segid 3A4 and resid 42 and name CB)	(segid 3A4 and resid 327 and name CA)	13.30	0.36	0.36
	assign (segid 3A4 and resid 42 and name CB)	(segid 3A4 and resid 327 and name CB)	13.62	0.47	0.47
75	assign (segid 3A4 and resid 42 and name CB)	(segid 3A4 and resid 328 and name CA)	13.15	0.44	0.44
	assign (segid 3A4 and resid 42 and name CB)	(segid 3A4 and resid 328 and name CB)	14.47	0.49	0.49
	assign (segid 3A4 and resid 42 and name CB)	(segid 3A4 and resid 329 and name CA)	10.55	0.67	0.68
	assign (segid 3A4 and resid 42 and name CB)	(segid 3A4 and resid 329 and name CB)	9.27	0.70	0.70
	assign (segid 3A4 and resid 42 and name CB)	(segid 3A4 and resid 330 and name CA)	10.68	0.57	0.57
80	assign (segid 3A4 and resid 42 and name CB)	(segid 3A4 and resid 330 and name CB)	12.02	0.58	0.58
	assign (segid 3A4 and resid 42 and name CB)	(segid 3A4 and resid 331 and name CA)	8.01	0.51	0.51
	assign (segid 3A4 and resid 42 and name CB)	(segid 3A4 and resid 331 and name CB)	6.82	0.53	0.52

5	assign	(segid 3A4 and resid 42 and name CB)	(segid 3A4 and resid 332 and name CA)	10.22	0.56	0.57
	assign	(segid 3A4 and resid 42 and name CB)	(segid 3A4 and resid 333 and name CA)	13.22	0.51	0.51
	assign	(segid 3A4 and resid 42 and name CB)	(segid 3A4 and resid 335 and name CA)	12.17	0.41	0.41
	assign	(segid 3A4 and resid 42 and name CB)	(segid 3A4 and resid 336 and name CA)	12.59	0.47	0.47
	assign	(segid 3A4 and resid 42 and name CB)	(segid 3A4 and resid 337 and name CA)	14.06	0.48	0.49
10	assign	(segid 3A4 and resid 42 and name CB)	(segid 3A4 and resid 337 and name CB)	10.89	0.34	0.33
	assign	(segid 3A4 and resid 42 and name CB)	(segid 3A4 and resid 337 and name CB)	9.12	0.34	0.33
	assign	(segid 3A4 and resid 42 and name CB)	(segid 3A4 and resid 338 and name CA)	13.57	0.22	0.22
	assign	(segid 3A4 and resid 42 and name CB)	(segid 3A4 and resid 338 and name CB)	14.78	0.30	0.30
	assign	(segid 3A4 and resid 42 and name CB)	(segid 3A4 and resid 339 and name CA)	13.82	0.23	0.23
15	assign	(segid 3A4 and resid 42 and name CB)	(segid 3A4 and resid 339 and name CB)	15.02	0.24	0.24
	assign	(segid 3A4 and resid 42 and name CB)	(segid 3A4 and resid 340 and name CA)	13.92	0.40	0.40
	assign	(segid 3A4 and resid 42 and name CB)	(segid 3A4 and resid 341 and name CA)	12.02	0.36	0.36
	assign	(segid 3A4 and resid 42 and name CB)	(segid 3A4 and resid 341 and name CB)	11.55	0.36	0.35
	assign	(segid 3A4 and resid 42 and name CB)	(segid 3A4 and resid 342 and name CA)	10.62	0.51	0.51
20	assign	(segid 3A4 and resid 42 and name CB)	(segid 3A4 and resid 343 and name CA)	7.54	0.47	0.46
	assign	(segid 3A4 and resid 42 and name CB)	(segid 3A4 and resid 343 and name CB)	6.21	0.49	0.50
	assign	(segid 3A4 and resid 42 and name CB)	(segid 3A4 and resid 344 and name CA)	8.28	0.57	0.57
	assign	(segid 3A4 and resid 42 and name CB)	(segid 3A4 and resid 344 and name CB)	9.71	0.56	0.55
	assign	(segid 3A4 and resid 42 and name CB)	(segid 3A4 and resid 345 and name CA)	6.60	0.66	0.66
25	assign	(segid 3A4 and resid 42 and name CB)	(segid 3A4 and resid 345 and name CB)	5.70	0.80	0.80
	assign	(segid 3A4 and resid 42 and name CB)	(segid 3A4 and resid 346 and name CA)	9.83	0.55	0.55
	assign	(segid 3A4 and resid 42 and name CB)	(segid 3A4 and resid 346 and name CB)	10.60	0.40	0.40
	assign	(segid 3A4 and resid 42 and name CB)	(segid 3A4 and resid 347 and name CA)	10.74	0.58	0.59
	assign	(segid 3A4 and resid 42 and name CB)	(segid 3A4 and resid 347 and name CB)	11.22	0.66	0.65
30	assign	(segid 3A4 and resid 42 and name CB)	(segid 3A4 and resid 348 and name CA)	14.10	0.58	0.59
	assign	(segid 3A4 and resid 42 and name CB)	(segid 3A4 and resid 349 and name CA)	13.15	0.33	0.33
	assign	(segid 3A4 and resid 42 and name CB)	(segid 3A4 and resid 349 and name CB)	12.44	0.32	0.32
	assign	(segid 3A4 and resid 42 and name CB)	(segid 3A4 and resid 350 and name CA)	11.58	0.47	0.46
	assign	(segid 3A4 and resid 42 and name CB)	(segid 3A4 and resid 350 and name CB)	10.53	0.57	0.57
35	assign	(segid 3A4 and resid 42 and name CB)	(segid 3A4 and resid 351 and name CA)	14.83	0.51	0.51
	assign	(segid 3A4 and resid 42 and name CB)	(segid 3A4 and resid 352 and name CA)	16.83	0.47	0.47
	assign	(segid 3A4 and resid 42 and name CB)	(segid 3A4 and resid 352 and name CB)	17.26	0.50	0.50
	assign	(segid 3A4 and resid 42 and name CB)	(segid 3A4 and resid 353 and name CA)	15.53	0.54	0.53
	assign	(segid 3A4 and resid 42 and name CB)	(segid 3A4 and resid 353 and name CB)	14.27	0.62	0.62
40	assign	(segid 3A4 and resid 42 and name CB)	(segid 3A4 and resid 355 and name CB)	16.86	1.03	1.04
	assign	(segid 3A4 and resid 42 and name CB)	(segid 3A4 and resid 356 and name CA)	17.07	0.81	0.81
	assign	(segid 3A4 and resid 42 and name CB)	(segid 3A4 and resid 356 and name CB)	15.74	0.79	0.80
	assign	(segid 3A4 and resid 42 and name CB)	(segid 3A4 and resid 381 and name CA)	14.82	0.71	0.71
	assign	(segid 3A4 and resid 42 and name CB)	(segid 3A4 and resid 382 and name CA)	12.18	0.52	0.51
45	assign	(segid 3A4 and resid 42 and name CB)	(segid 3A4 and resid 382 and name CB)	10.74	0.53	0.53
	assign	(segid 3A4 and resid 42 and name CB)	(segid 3A4 and resid 383 and name CA)	14.67	0.39	0.39
	assign	(segid 3A4 and resid 42 and name CB)	(segid 3A4 and resid 384 and name CA)	14.70	0.34	0.34
	assign	(segid 3A4 and resid 42 and name CB)	(segid 3A4 and resid 384 and name CB)	15.71	0.33	0.33
	assign	(segid 3A4 and resid 42 and name CB)	(segid 3A4 and resid 385 and name CA)	11.04	0.33	0.33
50	assign	(segid 3A4 and resid 42 and name CB)	(segid 3A4 and resid 386 and name CA)	9.76	0.24	0.24
	assign	(segid 3A4 and resid 42 and name CB)	(segid 3A4 and resid 387 and name CA)	9.99	0.82	0.83
	assign	(segid 3A4 and resid 42 and name CB)	(segid 3A4 and resid 388 and name CA)	12.38	0.92	0.92
	assign	(segid 3A4 and resid 42 and name CB)	(segid 3A4 and resid 388 and name CB)	12.51	1.11	1.10
	assign	(segid 3A4 and resid 42 and name CB)	(segid 3A4 and resid 389 and name CA)	12.38	0.52	0.53
55	assign	(segid 3A4 and resid 42 and name CB)	(segid 3A4 and resid 389 and name CB)	11.59	0.49	0.49
	assign	(segid 3A4 and resid 42 and name CB)	(segid 3A4 and resid 390 and name CA)	13.24	0.51	0.50
	assign	(segid 3A4 and resid 42 and name CB)	(segid 3A4 and resid 390 and name CB)	13.52	0.56	0.56
	assign	(segid 3A4 and resid 42 and name CB)	(segid 3A4 and resid 391 and name CA)	16.26	0.44	0.44
	assign	(segid 3A4 and resid 42 and name CB)	(segid 3A4 and resid 391 and name CB)	16.67	0.39	0.40
60	assign	(segid 3A4 and resid 42 and name CB)	(segid 3A4 and resid 392 and name CA)	19.29	0.51	0.51
	assign	(segid 3A4 and resid 42 and name CB)	(segid 3A4 and resid 68 and name CA)	16.48	1.32	1.32
	assign	(segid 3A4 and resid 42 and name CB)	(segid 3A4 and resid 69 and name CA)	16.70	1.23	1.24
	assign	(segid 3A4 and resid 42 and name CB)	(segid 3A4 and resid 70 and name CA)	17.01	1.25	1.25
	assign	(segid 3A4 and resid 42 and name CB)	(segid 3A4 and resid 71 and name CA)	15.47	1.56	1.56
65	assign	(segid 3A4 and resid 42 and name N)	(segid 3A4 and resid 42 and name CA)	1.45	0.01	0.01
	assign	(segid 3A4 and resid 42 and name N)	(segid 3A4 and resid 42 and name CB)	2.43	0.03	0.03
	assign	(segid 3A4 and resid 42 and name N)	(segid 3A4 and resid 42 and name O)	3.44	0.10	0.10
	assign	(segid 3A4 and resid 42 and name O)	(segid 3A4 and resid 42 and name CB)	3.34	0.11	0.11
	assign	(segid 3A4 and resid 430 and name C)	(segid 3A4 and resid 430 and name O)	1.23	0.00	0.00
70	assign	(segid 3A4 and resid 430 and name C)	(segid 3A4 and resid 431 and name C)	3.18	0.17	0.17
	assign	(segid 3A4 and resid 430 and name C)	(segid 3A4 and resid 431 and name CA)	2.44	0.02	0.03
	assign	(segid 3A4 and resid 430 and name C)	(segid 3A4 and resid 431 and name N)	1.34	0.02	0.01
	assign	(segid 3A4 and resid 430 and name C)	(segid 3A4 and resid 431 and name O)	3.77	0.22	0.21
	assign	(segid 3A4 and resid 430 and name C)	(segid 3A4 and resid 433 and name N)	5.91	0.65	0.64
75	assign	(segid 3A4 and resid 430 and name CA)	(segid 3A4 and resid 430 and name C)	1.52	0.01	0.01
	assign	(segid 3A4 and resid 430 and name CA)	(segid 3A4 and resid 430 and name O)	2.40	0.01	0.01
	assign	(segid 3A4 and resid 430 and name CA)	(segid 3A4 and resid 431 and name C)	4.46	0.15	0.15
	assign	(segid 3A4 and resid 430 and name CA)	(segid 3A4 and resid 431 and name CA)	3.81	0.03	0.04
	assign	(segid 3A4 and resid 430 and name CA)	(segid 3A4 and resid 431 and name N)	2.44	0.03	0.04
80	assign	(segid 3A4 and resid 430 and name CA)	(segid 3A4 and resid 431 and name O)	5.03	0.30	0.31
	assign	(segid 3A4 and resid 430 and name CA)	(segid 3A4 and resid 433 and name CA)	6.93	0.91	0.91
	assign	(segid 3A4 and resid 430 and name CA)	(segid 3A4 and resid 434 and name CA)	9.58	0.79	0.79
	assign	(segid 3A4 and resid 430 and name CA)	(segid 3A4 and resid 435 and name CA)	12.58	0.65	0.66
	assign	(segid 3A4 and resid 430 and name CA)	(segid 3A4 and resid 436 and name CA)	13.71	1.07	1.07
	assign	(segid 3A4 and resid 430 and name CA)	(segid 3A4 and resid 437 and name CA)	16.99	0.89	0.88

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	assign (segid 3A4 and resid 434 and name C)	(segid 3A4 and resid 436 and name O)	6.94	0.61	0.61
	assign (segid 3A4 and resid 434 and name C)	(segid 3A4 and resid 437 and name N)	6.89	0.15	0.15
	assign (segid 3A4 and resid 434 and name CA)	(segid 3A4 and resid 434 and name C)	1.53	0.01	0.00
	assign (segid 3A4 and resid 434 and name CA)	(segid 3A4 and resid 434 and name O)	2.39	0.02	0.02
5	assign (segid 3A4 and resid 434 and name CA)	(segid 3A4 and resid 435 and name C)	4.58	0.07	0.07
	assign (segid 3A4 and resid 434 and name CA)	(segid 3A4 and resid 435 and name CA)	3.83	0.04	0.04
	assign (segid 3A4 and resid 434 and name CA)	(segid 3A4 and resid 435 and name N)	2.45	0.07	0.07
	assign (segid 3A4 and resid 434 and name CA)	(segid 3A4 and resid 435 and name O)	4.75	0.21	0.22
	assign (segid 3A4 and resid 434 and name CA)	(segid 3A4 and resid 436 and name C)	7.58	0.22	0.23
10	assign (segid 3A4 and resid 434 and name CA)	(segid 3A4 and resid 436 and name CA)	6.55	0.18	0.18
	assign (segid 3A4 and resid 434 and name CA)	(segid 3A4 and resid 436 and name N)	5.48	0.15	0.15
	assign (segid 3A4 and resid 434 and name CA)	(segid 3A4 and resid 437 and name N)	9.32	0.11	0.12
	assign (segid 3A4 and resid 434 and name CA)	(segid 3A4 and resid 438 and name CA)	10.61	0.63	0.62
	assign (segid 3A4 and resid 434 and name CA)	(segid 3A4 and resid 439 and name CA)	14.25	0.61	0.61
15	assign (segid 3A4 and resid 434 and name CA)	(segid 3A4 and resid 440 and name CA)	16.34	0.55	0.55
	assign (segid 3A4 and resid 434 and name N)	(segid 3A4 and resid 434 and name C)	2.45	0.02	0.03
	assign (segid 3A4 and resid 434 and name N)	(segid 3A4 and resid 434 and name CA)	1.46	0.01	0.02
	assign (segid 3A4 and resid 434 and name N)	(segid 3A4 and resid 434 and name O)	2.70	0.07	0.07
	assign (segid 3A4 and resid 434 and name N)	(segid 3A4 and resid 435 and name C)	5.65	0.15	0.14
20	assign (segid 3A4 and resid 434 and name N)	(segid 3A4 and resid 435 and name CA)	4.88	0.05	0.06
	assign (segid 3A4 and resid 434 and name N)	(segid 3A4 and resid 435 and name N)	3.65	0.05	0.05
	assign (segid 3A4 and resid 434 and name N)	(segid 3A4 and resid 435 and name O)	5.93	0.28	0.28
	assign (segid 3A4 and resid 434 and name N)	(segid 3A4 and resid 436 and name CA)	7.41	0.29	0.29
	assign (segid 3A4 and resid 434 and name N)	(segid 3A4 and resid 436 and name N)	6.36	0.25	0.24
25	assign (segid 3A4 and resid 434 and name N)	(segid 3A4 and resid 435 and name C)	3.53	0.34	0.35
	assign (segid 3A4 and resid 434 and name O)	(segid 3A4 and resid 435 and name CA)	2.78	0.04	0.04
	assign (segid 3A4 and resid 434 and name O)	(segid 3A4 and resid 435 and name N)	2.25	0.02	0.01
	assign (segid 3A4 and resid 434 and name O)	(segid 3A4 and resid 435 and name O)	4.19	0.53	0.52
	assign (segid 3A4 and resid 434 and name O)	(segid 3A4 and resid 436 and name C)	6.38	0.45	0.44
30	assign (segid 3A4 and resid 434 and name O)	(segid 3A4 and resid 436 and name CA)	5.24	0.45	0.45
	assign (segid 3A4 and resid 434 and name O)	(segid 3A4 and resid 436 and name N)	4.04	0.37	0.37
	assign (segid 3A4 and resid 434 and name O)	(segid 3A4 and resid 437 and name N)	6.87	0.29	0.29
	assign (segid 3A4 and resid 435 and name C)	(segid 3A4 and resid 435 and name O)	1.24	0.02	0.01
	assign (segid 3A4 and resid 435 and name C)	(segid 3A4 and resid 436 and name C)	3.18	0.12	0.11
35	assign (segid 3A4 and resid 435 and name C)	(segid 3A4 and resid 436 and name CA)	2.44	0.01	0.02
	assign (segid 3A4 and resid 435 and name C)	(segid 3A4 and resid 436 and name N)	1.32	0.01	0.02
	assign (segid 3A4 and resid 435 and name C)	(segid 3A4 and resid 436 and name O)	3.78	0.46	0.47
	assign (segid 3A4 and resid 435 and name C)	(segid 3A4 and resid 437 and name C)	5.34	0.32	0.31
	assign (segid 3A4 and resid 435 and name C)	(segid 3A4 and resid 437 and name CA)	4.94	0.14	0.15
40	assign (segid 3A4 and resid 435 and name C)	(segid 3A4 and resid 437 and name N)	3.74	0.22	0.23
	assign (segid 3A4 and resid 435 and name C)	(segid 3A4 and resid 437 and name O)	5.52	0.59	0.59
	assign (segid 3A4 and resid 435 and name C)	(segid 3A4 and resid 438 and name CA)	6.68	0.61	0.61
	assign (segid 3A4 and resid 435 and name C)	(segid 3A4 and resid 438 and name N)	5.86	0.55	0.54
	assign (segid 3A4 and resid 435 and name C)	(segid 3A4 and resid 435 and name C)	1.52	0.00	0.00
45	assign (segid 3A4 and resid 435 and name CA)	(segid 3A4 and resid 435 and name O)	2.40	0.01	0.01
	assign (segid 3A4 and resid 435 and name CA)	(segid 3A4 and resid 436 and name C)	4.52	0.08	0.08
	assign (segid 3A4 and resid 435 and name CA)	(segid 3A4 and resid 436 and name CA)	3.81	0.01	0.02
	assign (segid 3A4 and resid 435 and name CA)	(segid 3A4 and resid 436 and name N)	2.44	0.03	0.02
	assign (segid 3A4 and resid 435 and name CA)	(segid 3A4 and resid 436 and name O)	5.10	0.54	0.54
50	assign (segid 3A4 and resid 435 and name CA)	(segid 3A4 and resid 437 and name C)	6.10	0.49	0.50
	assign (segid 3A4 and resid 435 and name CA)	(segid 3A4 and resid 437 and name CA)	6.00	0.28	0.28
	assign (segid 3A4 and resid 435 and name CA)	(segid 3A4 and resid 437 and name N)	4.89	0.36	0.36
	assign (segid 3A4 and resid 435 and name CA)	(segid 3A4 and resid 437 and name O)	6.10	0.89	0.89
	assign (segid 3A4 and resid 435 and name CA)	(segid 3A4 and resid 438 and name CA)	7.11	0.69	0.68
55	assign (segid 3A4 and resid 435 and name CA)	(segid 3A4 and resid 438 and name N)	6.54	0.55	0.55
	assign (segid 3A4 and resid 435 and name CA)	(segid 3A4 and resid 439 and name CA)	10.81	0.60	0.60
	assign (segid 3A4 and resid 435 and name CA)	(segid 3A4 and resid 440 and name CA)	13.09	0.52	0.53
	assign (segid 3A4 and resid 435 and name N)	(segid 3A4 and resid 435 and name C)	2.46	0.06	0.06
	assign (segid 3A4 and resid 435 and name N)	(segid 3A4 and resid 435 and name CA)	1.47	0.02	0.02
60	assign (segid 3A4 and resid 435 and name N)	(segid 3A4 and resid 435 and name O)	2.88	0.12	0.12
	assign (segid 3A4 and resid 435 and name N)	(segid 3A4 and resid 436 and name C)	5.60	0.14	0.14
	assign (segid 3A4 and resid 435 and name N)	(segid 3A4 and resid 436 and name CA)	4.77	0.09	0.09
	assign (segid 3A4 and resid 435 and name N)	(segid 3A4 and resid 436 and name N)	3.52	0.08	0.09
	assign (segid 3A4 and resid 435 and name N)	(segid 3A4 and resid 436 and name O)	6.10	0.56	0.57
65	assign (segid 3A4 and resid 435 and name N)	(segid 3A4 and resid 437 and name CA)	7.19	0.15	0.16
	assign (segid 3A4 and resid 435 and name N)	(segid 3A4 and resid 437 and name N)	6.09	0.25	0.24
	assign (segid 3A4 and resid 435 and name O)	(segid 3A4 and resid 436 and name C)	3.25	0.23	0.23
	assign (segid 3A4 and resid 435 and name O)	(segid 3A4 and resid 436 and name CA)	2.76	0.05	0.05
	assign (segid 3A4 and resid 435 and name O)	(segid 3A4 and resid 436 and name N)	2.24	0.03	0.02
70	assign (segid 3A4 and resid 435 and name O)	(segid 3A4 and resid 436 and name O)	3.66	0.48	0.49
	assign (segid 3A4 and resid 435 and name O)	(segid 3A4 and resid 437 and name C)	5.44	0.42	0.42
	assign (segid 3A4 and resid 435 and name O)	(segid 3A4 and resid 437 and name CA)	4.95	0.29	0.28
	assign (segid 3A4 and resid 435 and name O)	(segid 3A4 and resid 437 and name N)	3.88	0.27	0.27
	assign (segid 3A4 and resid 435 and name O)	(segid 3A4 and resid 437 and name O)	5.82	0.43	0.42
75	assign (segid 3A4 and resid 435 and name O)	(segid 3A4 and resid 438 and name CA)	6.71	0.87	0.86
	assign (segid 3A4 and resid 435 and name O)	(segid 3A4 and resid 438 and name N)	5.82	0.81	0.80
	assign (segid 3A4 and resid 436 and name C)	(segid 3A4 and resid 436 and name O)	1.23	0.00	0.01
	assign (segid 3A4 and resid 436 and name C)	(segid 3A4 and resid 437 and name C)	3.50	0.12	0.12
	assign (segid 3A4 and resid 436 and name C)	(segid 3A4 and resid 437 and name CA)	2.44	0.02	0.01
80	assign (segid 3A4 and resid 436 and name C)	(segid 3A4 and resid 437 and name N)	1.32	0.01	0.01
	assign (segid 3A4 and resid 436 and name C)	(segid 3A4 and resid 437 and name O)	4.05	0.16	0.16
	assign (segid 3A4 and resid 436 and name C)	(segid 3A4 and resid 438 and name C)	6.68	0.37	0.37
	assign (segid 3A4 and resid 436 and name C)	(segid 3A4 and resid 438 and name CA)	5.54	0.36	0.36

	assign (segid 3A4 and resid 436 and name C) (segid 3A4 and resid 438 and name N)	4.28	0.36	0.36
	assign (segid 3A4 and resid 436 and name C) (segid 3A4 and resid 438 and name O)	7.07	0.50	0.50
	assign (segid 3A4 and resid 436 and name C) (segid 3A4 and resid 439 and name N)	7.44	0.29	0.29
	assign (segid 3A4 and resid 436 and name CA) (segid 3A4 and resid 436 and name C)	1.53	0.01	0.00
	assign (segid 3A4 and resid 436 and name CA) (segid 3A4 and resid 436 and name O)	2.41	0.01	0.01
5	assign (segid 3A4 and resid 436 and name CA) (segid 3A4 and resid 437 and name C)	4.72	0.06	0.07
	assign (segid 3A4 and resid 436 and name CA) (segid 3A4 and resid 437 and name CA)	3.82	0.02	0.02
	assign (segid 3A4 and resid 436 and name CA) (segid 3A4 and resid 437 and name N)	2.44	0.02	0.03
	assign (segid 3A4 and resid 436 and name CA) (segid 3A4 and resid 437 and name O)	5.03	0.32	0.32
	assign (segid 3A4 and resid 436 and name CA) (segid 3A4 and resid 438 and name CA)	6.67	0.35	0.34
10	assign (segid 3A4 and resid 436 and name CA) (segid 3A4 and resid 438 and name N)	5.52	0.36	0.37
	assign (segid 3A4 and resid 436 and name CA) (segid 3A4 and resid 439 and name N)	9.99	0.31	0.31
	assign (segid 3A4 and resid 436 and name CA) (segid 3A4 and resid 440 and name CA)	12.98	0.22	0.22
	assign (segid 3A4 and resid 436 and name N) (segid 3A4 and resid 436 and name C)	2.46	0.04	0.04
	assign (segid 3A4 and resid 436 and name N) (segid 3A4 and resid 436 and name CA)	1.46	0.01	0.01
15	assign (segid 3A4 and resid 436 and name N) (segid 3A4 and resid 436 and name O)	3.27	0.33	0.33
	assign (segid 3A4 and resid 436 and name N) (segid 3A4 and resid 437 and name C)	4.98	0.24	0.24
	assign (segid 3A4 and resid 436 and name N) (segid 3A4 and resid 437 and name CA)	4.43	0.21	0.20
	assign (segid 3A4 and resid 436 and name N) (segid 3A4 and resid 437 and name N)	3.07	0.28	0.29
	assign (segid 3A4 and resid 436 and name N) (segid 3A4 and resid 437 and name O)	5.11	0.58	0.59
20	assign (segid 3A4 and resid 436 and name N) (segid 3A4 and resid 438 and name CA)	6.64	0.33	0.34
	assign (segid 3A4 and resid 436 and name N) (segid 3A4 and resid 438 and name N)	5.71	0.35	0.35
	assign (segid 3A4 and resid 436 and name N) (segid 3A4 and resid 437 and name C)	3.87	0.27	0.27
	assign (segid 3A4 and resid 436 and name O) (segid 3A4 and resid 437 and name CA)	2.74	0.04	0.03
	assign (segid 3A4 and resid 436 and name O) (segid 3A4 and resid 437 and name N)	2.22	0.02	0.02
25	assign (segid 3A4 and resid 436 and name O) (segid 3A4 and resid 437 and name O)	4.61	0.24	0.24
	assign (segid 3A4 and resid 436 and name O) (segid 3A4 and resid 438 and name C)	6.76	0.46	0.47
	assign (segid 3A4 and resid 436 and name O) (segid 3A4 and resid 438 and name CA)	5.75	0.53	0.52
	assign (segid 3A4 and resid 436 and name O) (segid 3A4 and resid 438 and name N)	4.44	0.44	0.44
	assign (segid 3A4 and resid 436 and name O) (segid 3A4 and resid 437 and name C)	1.24	0.01	0.00
30	assign (segid 3A4 and resid 437 and name C) (segid 3A4 and resid 438 and name C)	3.48	0.18	0.18
	assign (segid 3A4 and resid 437 and name C) (segid 3A4 and resid 438 and name CA)	2.41	0.02	0.02
	assign (segid 3A4 and resid 437 and name C) (segid 3A4 and resid 438 and name N)	1.33	0.02	0.01
	assign (segid 3A4 and resid 437 and name C) (segid 3A4 and resid 438 and name O)	4.16	0.27	0.28
	assign (segid 3A4 and resid 437 and name C) (segid 3A4 and resid 439 and name C)	6.48	0.24	0.24
35	assign (segid 3A4 and resid 437 and name C) (segid 3A4 and resid 439 and name CA)	5.43	0.28	0.28
	assign (segid 3A4 and resid 437 and name C) (segid 3A4 and resid 439 and name N)	4.10	0.25	0.25
	assign (segid 3A4 and resid 437 and name C) (segid 3A4 and resid 439 and name O)	6.69	0.23	0.23
	assign (segid 3A4 and resid 437 and name CA) (segid 3A4 and resid 437 and name C)	1.51	0.01	0.01
	assign (segid 3A4 and resid 437 and name CA) (segid 3A4 and resid 437 and name O)	2.39	0.02	0.01
40	assign (segid 3A4 and resid 437 and name CA) (segid 3A4 and resid 438 and name C)	4.68	0.13	0.14
	assign (segid 3A4 and resid 437 and name CA) (segid 3A4 and resid 438 and name CA)	3.78	0.02	0.02
	assign (segid 3A4 and resid 437 and name CA) (segid 3A4 and resid 438 and name N)	2.43	0.02	0.01
	assign (segid 3A4 and resid 437 and name CA) (segid 3A4 and resid 438 and name O)	5.16	0.29	0.28
	assign (segid 3A4 and resid 437 and name CA) (segid 3A4 and resid 439 and name CA)	6.50	0.27	0.28
45	assign (segid 3A4 and resid 437 and name CA) (segid 3A4 and resid 439 and name N)	5.31	0.25	0.25
	assign (segid 3A4 and resid 437 and name CA) (segid 3A4 and resid 440 and name CA)	9.79	0.24	0.25
	assign (segid 3A4 and resid 437 and name N) (segid 3A4 and resid 437 and name C)	2.43	0.03	0.02
	assign (segid 3A4 and resid 437 and name N) (segid 3A4 and resid 437 and name CA)	1.46	0.01	0.02
	assign (segid 3A4 and resid 437 and name N) (segid 3A4 and resid 437 and name O)	2.90	0.27	0.27
50	assign (segid 3A4 and resid 437 and name N) (segid 3A4 and resid 438 and name C)	5.76	0.28	0.28
	assign (segid 3A4 and resid 437 and name N) (segid 3A4 and resid 438 and name CA)	4.64	0.17	0.16
	assign (segid 3A4 and resid 437 and name N) (segid 3A4 and resid 438 and name N)	3.39	0.23	0.23
	assign (segid 3A4 and resid 437 and name N) (segid 3A4 and resid 438 and name O)	6.24	0.45	0.44
	assign (segid 3A4 and resid 437 and name N) (segid 3A4 and resid 439 and name N)	6.45	0.26	0.26
55	assign (segid 3A4 and resid 437 and name N) (segid 3A4 and resid 438 and name C)	3.88	0.32	0.31
	assign (segid 3A4 and resid 437 and name O) (segid 3A4 and resid 438 and name CA)	2.73	0.03	0.02
	assign (segid 3A4 and resid 437 and name O) (segid 3A4 and resid 438 and name N)	2.24	0.01	0.01
	assign (segid 3A4 and resid 437 and name O) (segid 3A4 and resid 438 and name O)	4.75	0.37	0.37
60	assign (segid 3A4 and resid 437 and name O) (segid 3A4 and resid 439 and name C)	6.58	0.48	0.48
	assign (segid 3A4 and resid 437 and name O) (segid 3A4 and resid 439 and name CA)	5.63	0.53	0.53
	assign (segid 3A4 and resid 437 and name O) (segid 3A4 and resid 439 and name N)	4.26	0.44	0.44
	assign (segid 3A4 and resid 437 and name O) (segid 3A4 and resid 439 and name O)	6.59	0.46	0.47
	assign (segid 3A4 and resid 438 and name C) (segid 3A4 and resid 438 and name O)	1.23	0.00	0.00
65	assign (segid 3A4 and resid 438 and name C) (segid 3A4 and resid 439 and name C)	3.23	0.13	0.13
	assign (segid 3A4 and resid 438 and name C) (segid 3A4 and resid 439 and name CA)	2.45	0.01	0.01
	assign (segid 3A4 and resid 438 and name C) (segid 3A4 and resid 439 and name N)	1.34	0.01	0.00
	assign (segid 3A4 and resid 438 and name C) (segid 3A4 and resid 439 and name O)	3.67	0.09	0.09
	assign (segid 3A4 and resid 438 and name C) (segid 3A4 and resid 440 and name C)	6.44	0.22	0.23
70	assign (segid 3A4 and resid 438 and name C) (segid 3A4 and resid 440 and name CA)	5.19	0.26	0.26
	assign (segid 3A4 and resid 438 and name C) (segid 3A4 and resid 440 and name N)	4.02	0.25	0.25
	assign (segid 3A4 and resid 438 and name C) (segid 3A4 and resid 440 and name O)	6.57	0.20	0.19
	assign (segid 3A4 and resid 438 and name CA) (segid 3A4 and resid 438 and name C)	1.53	0.01	0.02
	assign (segid 3A4 and resid 438 and name CA) (segid 3A4 and resid 439 and name C)	2.40	0.02	0.02
75	assign (segid 3A4 and resid 438 and name CA) (segid 3A4 and resid 439 and name CA)	3.83	0.01	0.02
	assign (segid 3A4 and resid 438 and name CA) (segid 3A4 and resid 439 and name N)	2.45	0.03	0.02
	assign (segid 3A4 and resid 438 and name CA) (segid 3A4 and resid 439 and name O)	4.69	0.06	0.05
	assign (segid 3A4 and resid 438 and name CA) (segid 3A4 and resid 440 and name CA)	6.45	0.19	0.20
80	assign (segid 3A4 and resid 438 and name CA) (segid 3A4 and resid 440 and name N)	5.41	0.19	0.20
	assign (segid 3A4 and resid 438 and name N) (segid 3A4 and resid 438 and name C)	2.42	0.05	0.05
	assign (segid 3A4 and resid 438 and name N) (segid 3A4 and resid 438 and name CA)	1.45	0.01	0.01
	assign (segid 3A4 and resid 438 and name N) (segid 3A4 and resid 438 and name O)	2.98	0.14	0.15

	assign (segid 3A4 and resid 438 and name N)	(segid 3A4 and resid 439 and name C)	5.58	0.13	0.13
	assign (segid 3A4 and resid 438 and name N)	(segid 3A4 and resid 439 and name CA)	1.60	0.10	0.11
	assign (segid 3A4 and resid 438 and name N)	(segid 3A4 and resid 439 and name N)	3.30	0.13	0.14
	assign (segid 3A4 and resid 438 and name N)	(segid 3A4 and resid 439 and name O)	5.89	0.05	0.05
5	assign (segid 3A4 and resid 438 and name N)	(segid 3A4 and resid 440 and name CA)	7.57	0.24	0.25
	assign (segid 3A4 and resid 438 and name N)	(segid 3A4 and resid 440 and name N)	6.41	0.25	0.25
	assign (segid 3A4 and resid 438 and name N)	(segid 3A4 and resid 439 and name C)	3.42	0.27	0.28
	assign (segid 3A4 and resid 438 and name O)	(segid 3A4 and resid 439 and name CA)	2.78	0.03	0.03
	assign (segid 3A4 and resid 438 and name O)	(segid 3A4 and resid 439 and name N)	2.25	0.02	0.02
	assign (segid 3A4 and resid 438 and name O)	(segid 3A4 and resid 439 and name O)	4.12	0.26	0.25
10	assign (segid 3A4 and resid 438 and name O)	(segid 3A4 and resid 440 and name C)	6.15	0.44	0.44
	assign (segid 3A4 and resid 438 and name O)	(segid 3A4 and resid 440 and name CA)	4.98	0.53	0.52
	assign (segid 3A4 and resid 438 and name O)	(segid 3A4 and resid 440 and name N)	3.83	0.45	0.45
	assign (segid 3A4 and resid 438 and name O)	(segid 3A4 and resid 440 and name O)	6.17	0.34	0.35
	assign (segid 3A4 and resid 438 and name O)	(segid 3A4 and resid 440 and name O)	1.23	0.01	0.01
15	assign (segid 3A4 and resid 439 and name C)	(segid 3A4 and resid 440 and name C)	3.55	0.06	0.05
	assign (segid 3A4 and resid 439 and name C)	(segid 3A4 and resid 440 and name CA)	2.42	0.02	0.02
	assign (segid 3A4 and resid 439 and name C)	(segid 3A4 and resid 440 and name N)	1.32	0.01	0.01
	assign (segid 3A4 and resid 439 and name C)	(segid 3A4 and resid 440 and name O)	3.83	0.10	0.11
	assign (segid 3A4 and resid 439 and name C)	(segid 3A4 and resid 440 and name O)	1.51	0.01	0.01
20	assign (segid 3A4 and resid 439 and name CA)	(segid 3A4 and resid 439 and name C)	2.39	0.01	0.01
	assign (segid 3A4 and resid 439 and name CA)	(segid 3A4 and resid 439 and name O)	4.74	0.07	0.06
	assign (segid 3A4 and resid 439 and name CA)	(segid 3A4 and resid 440 and name CA)	3.79	0.02	0.03
	assign (segid 3A4 and resid 439 and name CA)	(segid 3A4 and resid 440 and name N)	2.43	0.02	0.02
	assign (segid 3A4 and resid 439 and name CA)	(segid 3A4 and resid 440 and name O)	4.71	0.13	0.13
25	assign (segid 3A4 and resid 439 and name N)	(segid 3A4 and resid 439 and name C)	2.44	0.04	0.03
	assign (segid 3A4 and resid 439 and name N)	(segid 3A4 and resid 439 and name CA)	1.47	0.02	0.01
	assign (segid 3A4 and resid 439 and name N)	(segid 3A4 and resid 439 and name O)	2.83	0.11	0.11
	assign (segid 3A4 and resid 439 and name N)	(segid 3A4 and resid 440 and name C)	5.91	0.05	0.05
	assign (segid 3A4 and resid 439 and name N)	(segid 3A4 and resid 440 and name CA)	4.73	0.02	0.03
30	assign (segid 3A4 and resid 439 and name N)	(segid 3A4 and resid 440 and name N)	3.50	0.03	0.03
	assign (segid 3A4 and resid 439 and name N)	(segid 3A4 and resid 440 and name O)	6.02	0.11	0.11
	assign (segid 3A4 and resid 439 and name O)	(segid 3A4 and resid 440 and name C)	3.97	0.09	0.08
	assign (segid 3A4 and resid 439 and name O)	(segid 3A4 and resid 440 and name CA)	2.74	0.03	0.03
	assign (segid 3A4 and resid 439 and name O)	(segid 3A4 and resid 440 and name N)	2.23	0.02	0.01
35	assign (segid 3A4 and resid 439 and name O)	(segid 3A4 and resid 440 and name O)	4.53	0.12	0.13
	assign (segid 3A4 and resid 440 and name C)	(segid 3A4 and resid 440 and name O)	1.23	0.01	0.01
	assign (segid 3A4 and resid 440 and name CA)	(segid 3A4 and resid 440 and name C)	1.53	0.02	0.02
	assign (segid 3A4 and resid 440 and name CA)	(segid 3A4 and resid 440 and name O)	2.40	0.03	0.03
40	assign (segid 3A4 and resid 440 and name N)	(segid 3A4 and resid 440 and name C)	2.44	0.04	0.05
	assign (segid 3A4 and resid 440 and name N)	(segid 3A4 and resid 440 and name CA)	1.45	0.00	0.00
	assign (segid 3A4 and resid 440 and name N)	(segid 3A4 and resid 440 and name O)	2.69	0.09	0.09
	assign (segid 3A4 and resid 440 and name N)	(segid 3A4 and resid 54 and name CB)	2.49	0.02	0.03
	assign (segid 3A4 and resid 54 and name C)	(segid 3A4 and resid 54 and name O)	1.23	0.01	0.01
45	assign (segid 3A4 and resid 54 and name C)	(segid 3A4 and resid 55 and name C)	3.11	0.21	0.21
	assign (segid 3A4 and resid 54 and name C)	(segid 3A4 and resid 55 and name CA)	2.43	0.02	0.02
	assign (segid 3A4 and resid 54 and name C)	(segid 3A4 and resid 55 and name CB)	3.65	0.09	0.09
	assign (segid 3A4 and resid 54 and name C)	(segid 3A4 and resid 55 and name N)	1.33	0.00	0.00
	assign (segid 3A4 and resid 54 and name C)	(segid 3A4 and resid 55 and name O)	3.89	0.18	0.18
50	assign (segid 3A4 and resid 54 and name C)	(segid 3A4 and resid 56 and name C)	4.87	0.50	0.49
	assign (segid 3A4 and resid 54 and name C)	(segid 3A4 and resid 56 and name CA)	4.66	0.42	0.41
	assign (segid 3A4 and resid 54 and name C)	(segid 3A4 and resid 56 and name CB)	5.28	0.40	0.40
	assign (segid 3A4 and resid 54 and name C)	(segid 3A4 and resid 56 and name N)	3.45	0.36	0.36
	assign (segid 3A4 and resid 54 and name C)	(segid 3A4 and resid 56 and name O)	5.89	0.39	0.38
	assign (segid 3A4 and resid 54 and name C)	(segid 3A4 and resid 57 and name C)	5.33	0.73	0.72
55	assign (segid 3A4 and resid 54 and name C)	(segid 3A4 and resid 57 and name CA)	5.02	0.71	0.71
	assign (segid 3A4 and resid 54 and name C)	(segid 3A4 and resid 57 and name N)	4.24	0.70	0.70
	assign (segid 3A4 and resid 54 and name C)	(segid 3A4 and resid 58 and name C)	6.49	0.54	0.54
	assign (segid 3A4 and resid 54 and name C)	(segid 3A4 and resid 58 and name CA)	5.45	0.67	0.67
	assign (segid 3A4 and resid 54 and name C)	(segid 3A4 and resid 58 and name N)	4.58	0.72	0.73
60	assign (segid 3A4 and resid 54 and name C)	(segid 3A4 and resid 58 and name O)	7.43	0.17	0.16
	assign (segid 3A4 and resid 54 and name CA)	(segid 3A4 and resid 160 and name CA)	14.55	2.40	2.41
	assign (segid 3A4 and resid 54 and name CA)	(segid 3A4 and resid 161 and name CA)	15.30	1.70	1.69
	assign (segid 3A4 and resid 54 and name CA)	(segid 3A4 and resid 161 and name CB)	16.37	1.63	1.63
	assign (segid 3A4 and resid 54 and name CA)	(segid 3A4 and resid 187 and name CB)	14.14	3.07	3.08
65	assign (segid 3A4 and resid 54 and name CA)	(segid 3A4 and resid 322 and name CA)	11.60	3.27	3.28
	assign (segid 3A4 and resid 54 and name CA)	(segid 3A4 and resid 324 and name CA)	13.58	2.97	2.96
	assign (segid 3A4 and resid 54 and name CA)	(segid 3A4 and resid 324 and name CB)	12.91	2.95	2.95
	assign (segid 3A4 and resid 54 and name CA)	(segid 3A4 and resid 342 and name CA)	12.10	3.17	3.18
	assign (segid 3A4 and resid 54 and name CA)	(segid 3A4 and resid 431 and name CA)	13.29	2.29	2.30
70	assign (segid 3A4 and resid 54 and name CA)	(segid 3A4 and resid 54 and name C)	1.52	0.01	0.01
	assign (segid 3A4 and resid 54 and name CA)	(segid 3A4 and resid 54 and name CB)	1.52	0.01	0.01
	assign (segid 3A4 and resid 54 and name CA)	(segid 3A4 and resid 54 and name O)	2.39	0.02	0.01
	assign (segid 3A4 and resid 54 and name CA)	(segid 3A4 and resid 55 and name C)	4.52	0.18	0.18
	assign (segid 3A4 and resid 54 and name CA)	(segid 3A4 and resid 55 and name CA)	3.81	0.03	0.03
75	assign (segid 3A4 and resid 54 and name CA)	(segid 3A4 and resid 55 and name CB)	4.82	0.06	0.06
	assign (segid 3A4 and resid 54 and name CA)	(segid 3A4 and resid 55 and name N)	2.44	0.02	0.01
	assign (segid 3A4 and resid 54 and name CA)	(segid 3A4 and resid 55 and name O)	5.36	0.16	0.16
	assign (segid 3A4 and resid 54 and name CA)	(segid 3A4 and resid 56 and name C)	5.94	0.51	0.51
	assign (segid 3A4 and resid 54 and name CA)	(segid 3A4 and resid 56 and name CA)	5.73	0.11	0.40
80	assign (segid 3A4 and resid 54 and name CA)	(segid 3A4 and resid 56 and name CB)	6.03	0.40	0.39
	assign (segid 3A4 and resid 54 and name CA)	(segid 3A4 and resid 56 and name N)	4.61	0.33	0.33
	assign (segid 3A4 and resid 54 and name CA)	(segid 3A4 and resid 57 and name CA)	5.80	0.76	0.76

	assign (segid 3A4 and resid 54 and name CA) (segid 3A4 and resid 57 and name N)	5.14	0.71	0.71
	assign (segid 3A4 and resid 51 and name CA) (segid 3A4 and resid 58 and name CA)	6.66	0.73	0.72
	assign (segid 3A4 and resid 54 and name CA) (segid 3A4 and resid 58 and name N)	5.73	0.76	0.77
	assign (segid 3A4 and resid 54 and name CA) (segid 3A4 and resid 59 and name CA)	9.17	0.76	0.77
5	assign (segid 3A4 and resid 54 and name CA) (segid 3A4 and resid 59 and name CB)	9.21	0.74	0.75
	assign (segid 3A4 and resid 54 and name CA) (segid 3A4 and resid 68 and name CA)	15.73	2.80	2.80
	assign (segid 3A4 and resid 54 and name CA) (segid 3A4 and resid 69 and name CA)	13.71	3.21	3.21
	assign (segid 3A4 and resid 54 and name CA) (segid 3A4 and resid 161 and name CA)	14.95	1.74	1.74
	assign (segid 3A4 and resid 54 and name CB) (segid 3A4 and resid 161 and name CB)	16.06	1.70	1.71
10	assign (segid 3A4 and resid 54 and name CB) (segid 3A4 and resid 187 and name CB)	13.95	3.10	3.09
	assign (segid 3A4 and resid 54 and name CB) (segid 3A4 and resid 324 and name CB)	13.96	3.20	3.19
	assign (segid 3A4 and resid 54 and name CB) (segid 3A4 and resid 431 and name CA)	13.06	2.65	2.65
	assign (segid 3A4 and resid 54 and name CB) (segid 3A4 and resid 55 and name C)	4.87	0.17	0.18
	assign (segid 3A4 and resid 54 and name CB) (segid 3A4 and resid 55 and name CA)	4.46	0.09	0.08
15	assign (segid 3A4 and resid 54 and name CB) (segid 3A4 and resid 55 and name CB)	5.36	0.14	0.14
	assign (segid 3A4 and resid 54 and name CB) (segid 3A4 and resid 55 and name N)	3.11	0.08	0.09
	assign (segid 3A4 and resid 54 and name CB) (segid 3A4 and resid 55 and name O)	5.82	0.14	0.14
	assign (segid 3A4 and resid 54 and name CB) (segid 3A4 and resid 56 and name C)	5.82	0.49	0.48
	assign (segid 3A4 and resid 54 and name CB) (segid 3A4 and resid 56 and name CA)	5.50	0.45	0.45
20	assign (segid 3A4 and resid 54 and name CB) (segid 3A4 and resid 56 and name CB)	5.43	0.48	0.48
	assign (segid 3A4 and resid 54 and name CB) (segid 3A4 and resid 56 and name N)	4.58	0.38	0.37
	assign (segid 3A4 and resid 54 and name CB) (segid 3A4 and resid 56 and name O)	6.98	0.43	0.42
	assign (segid 3A4 and resid 54 and name CB) (segid 3A4 and resid 57 and name C)	6.60	0.53	0.54
	assign (segid 3A4 and resid 54 and name CB) (segid 3A4 and resid 57 and name CA)	5.78	0.57	0.57
25	assign (segid 3A4 and resid 54 and name CB) (segid 3A4 and resid 57 and name N)	5.02	0.58	0.59
	assign (segid 3A4 and resid 54 and name CB) (segid 3A4 and resid 58 and name CA)	7.40	0.48	0.48
	assign (segid 3A4 and resid 54 and name CB) (segid 3A4 and resid 58 and name N)	6.28	0.53	0.52
	assign (segid 3A4 and resid 54 and name CB) (segid 3A4 and resid 59 and name CA)	9.60	0.63	0.63
	assign (segid 3A4 and resid 54 and name CB) (segid 3A4 and resid 59 and name CB)	9.48	0.61	0.62
30	assign (segid 3A4 and resid 54 and name CB) (segid 3A4 and resid 68 and name CA)	16.13	3.28	3.28
	assign (segid 3A4 and resid 54 and name CB) (segid 3A4 and resid 69 and name CA)	14.30	3.62	3.63
	assign (segid 3A4 and resid 54 and name N) (segid 3A4 and resid 54 and name C)	2.44	0.04	0.04
	assign (segid 3A4 and resid 54 and name N) (segid 3A4 and resid 54 and name CA)	1.47	0.01	0.01
	assign (segid 3A4 and resid 54 and name N) (segid 3A4 and resid 54 and name CB)	2.41	0.04	0.04
	assign (segid 3A4 and resid 54 and name N) (segid 3A4 and resid 54 and name O)	2.67	0.06	0.06
35	assign (segid 3A4 and resid 54 and name N) (segid 3A4 and resid 55 and name C)	5.43	0.28	0.28
	assign (segid 3A4 and resid 54 and name N) (segid 3A4 and resid 55 and name CA)	4.85	0.06	0.06
	assign (segid 3A4 and resid 54 and name N) (segid 3A4 and resid 55 and name CB)	6.00	0.12	0.11
	assign (segid 3A4 and resid 54 and name N) (segid 3A4 and resid 55 and name N)	3.65	0.03	0.03
40	assign (segid 3A4 and resid 54 and name N) (segid 3A4 and resid 55 and name O)	6.06	0.29	0.29
	assign (segid 3A4 and resid 54 and name O) (segid 3A4 and resid 56 and name N)	5.59	0.45	0.46
	assign (segid 3A4 and resid 54 and name O) (segid 3A4 and resid 56 and name CB)	3.29	0.05	0.05
	assign (segid 3A4 and resid 54 and name O) (segid 3A4 and resid 55 and name C)	3.03	0.34	0.34
	assign (segid 3A4 and resid 54 and name O) (segid 3A4 and resid 55 and name CA)	2.75	0.03	0.04
45	assign (segid 3A4 and resid 54 and name O) (segid 3A4 and resid 55 and name CB)	4.14	0.17	0.16
	assign (segid 3A4 and resid 54 and name O) (segid 3A4 and resid 55 and name N)	2.24	0.01	0.02
	assign (segid 3A4 and resid 54 and name O) (segid 3A4 and resid 55 and name O)	3.47	0.33	0.33
	assign (segid 3A4 and resid 54 and name O) (segid 3A4 and resid 56 and name C)	4.37	0.78	0.77
	assign (segid 3A4 and resid 54 and name O) (segid 3A4 and resid 56 and name CA)	4.51	0.66	0.65
50	assign (segid 3A4 and resid 54 and name O) (segid 3A4 and resid 56 and name CB)	5.32	0.65	0.64
	assign (segid 3A4 and resid 54 and name O) (segid 3A4 and resid 56 and name N)	3.53	0.54	0.54
	assign (segid 3A4 and resid 54 and name O) (segid 3A4 and resid 56 and name O)	5.25	0.65	0.66
	assign (segid 3A4 and resid 54 and name O) (segid 3A4 and resid 57 and name C)	4.33	1.04	1.05
	assign (segid 3A4 and resid 54 and name O) (segid 3A4 and resid 57 and name CA)	4.20	1.05	1.05
55	assign (segid 3A4 and resid 54 and name O) (segid 3A4 and resid 57 and name N)	3.64	1.03	1.03
	assign (segid 3A4 and resid 54 and name O) (segid 3A4 and resid 58 and name C)	5.55	0.75	0.76
	assign (segid 3A4 and resid 54 and name O) (segid 3A4 and resid 58 and name CA)	4.46	0.87	0.87
	assign (segid 3A4 and resid 54 and name O) (segid 3A4 and resid 58 and name N)	3.57	1.01	1.01
	assign (segid 3A4 and resid 54 and name O) (segid 3A4 and resid 58 and name O)	6.47	0.36	0.36
60	assign (segid 3A4 and resid 55 and name C) (segid 3A4 and resid 55 and name CB)	2.48	0.02	0.03
	assign (segid 3A4 and resid 55 and name C) (segid 3A4 and resid 55 and name O)	1.23	0.00	0.01
	assign (segid 3A4 and resid 55 and name C) (segid 3A4 and resid 56 and name C)	2.99	0.04	0.03
	assign (segid 3A4 and resid 55 and name C) (segid 3A4 and resid 56 and name CA)	2.45	0.02	0.01
	assign (segid 3A4 and resid 55 and name C) (segid 3A4 and resid 56 and name CB)	3.69	0.04	0.05
65	assign (segid 3A4 and resid 55 and name C) (segid 3A4 and resid 56 and name N)	1.33	0.01	0.01
	assign (segid 3A4 and resid 55 and name C) (segid 3A4 and resid 56 and name O)	3.77	0.13	0.12
	assign (segid 3A4 and resid 55 and name C) (segid 3A4 and resid 57 and name C)	4.50	0.15	0.14
	assign (segid 3A4 and resid 55 and name C) (segid 3A4 and resid 57 and name CA)	4.41	0.10	0.11
	assign (segid 3A4 and resid 55 and name C) (segid 3A4 and resid 57 and name N)	3.26	0.11	0.11
70	assign (segid 3A4 and resid 55 and name C) (segid 3A4 and resid 57 and name O)	5.61	0.18	0.18
	assign (segid 3A4 and resid 55 and name C) (segid 3A4 and resid 58 and name C)	4.85	0.11	0.10
	assign (segid 3A4 and resid 55 and name C) (segid 3A4 and resid 58 and name CA)	4.49	0.12	0.12
	assign (segid 3A4 and resid 55 and name C) (segid 3A4 and resid 58 and name N)	3.73	0.12	0.12
	assign (segid 3A4 and resid 55 and name C) (segid 3A4 and resid 58 and name O)	5.83	0.35	0.35
75	assign (segid 3A4 and resid 55 and name C) (segid 3A4 and resid 59 and name C)	6.47	0.56	0.56
	assign (segid 3A4 and resid 55 and name C) (segid 3A4 and resid 59 and name CA)	5.29	0.46	0.45
	assign (segid 3A4 and resid 55 and name C) (segid 3A4 and resid 59 and name CB)	4.96	0.53	0.54
	assign (segid 3A4 and resid 55 and name C) (segid 3A4 and resid 59 and name N)	4.40	0.51	0.51
80	assign (segid 3A4 and resid 55 and name CA) (segid 3A4 and resid 161 and name CA)	16.04	2.21	2.20
	assign (segid 3A4 and resid 55 and name CA) (segid 3A4 and resid 187 and name CA)	14.95	2.33	2.32
	assign (segid 3A4 and resid 55 and name CA) (segid 3A4 and resid 187 and name CB)	13.80	2.26	2.26
	assign (segid 3A4 and resid 55 and name CA) (segid 3A4 and resid 322 and name CA)	13.45	2.40	2.40
	assign (segid 3A4 and resid 55 and name CA) (segid 3A4 and resid 323 and name CA)	14.59	2.37	2.38

	assign (segid 3A4 and resid 55 and name CA) (segid 3A4 and resid 324 and name CA)	14.32	2.41	2.41
	assign (segid 3A4 and resid 55 and name CA) (segid 3A4 and resid 324 and name CB)	13.12	2.41	2.40
	assign (segid 3A4 and resid 55 and name CA) (segid 3A4 and resid 340 and name CA)	15.36	2.82	2.82
	assign (segid 3A4 and resid 55 and name CA) (segid 3A4 and resid 342 and name CA)	13.14	2.87	2.87
	assign (segid 3A4 and resid 55 and name CA) (segid 3A4 and resid 431 and name CA)	15.31	2.14	2.15
5	assign (segid 3A4 and resid 55 and name CA) (segid 3A4 and resid 55 and name C)	1.52	0.00	0.01
	assign (segid 3A4 and resid 55 and name CA) (segid 3A4 and resid 55 and name CB)	1.52	0.01	0.02
	assign (segid 3A4 and resid 55 and name CA) (segid 3A4 and resid 55 and name O)	2.39	0.02	0.01
	assign (segid 3A4 and resid 55 and name CA) (segid 3A4 and resid 56 and name C)	4.42	0.02	0.03
	assign (segid 3A4 and resid 55 and name CA) (segid 3A4 and resid 56 and name CB)	3.82	0.03	0.03
10	assign (segid 3A4 and resid 55 and name CA) (segid 3A4 and resid 56 and name CB)	4.84	0.08	0.08
	assign (segid 3A4 and resid 55 and name CA) (segid 3A4 and resid 56 and name N)	2.44	0.04	0.04
	assign (segid 3A4 and resid 55 and name CA) (segid 3A4 and resid 56 and name O)	5.25	0.12	0.11
	assign (segid 3A4 and resid 55 and name CA) (segid 3A4 and resid 57 and name C)	5.51	0.21	0.21
	assign (segid 3A4 and resid 55 and name CA) (segid 3A4 and resid 57 and name CB)	5.49	0.15	0.15
15	assign (segid 3A4 and resid 55 and name CA) (segid 3A4 and resid 57 and name N)	4.44	0.16	0.16
	assign (segid 3A4 and resid 55 and name CA) (segid 3A4 and resid 57 and name O)	6.65	0.23	0.23
	assign (segid 3A4 and resid 55 and name CA) (segid 3A4 and resid 58 and name C)	5.71	0.19	0.19
	assign (segid 3A4 and resid 55 and name CA) (segid 3A4 and resid 58 and name CB)	5.13	0.26	0.25
	assign (segid 3A4 and resid 55 and name CA) (segid 3A4 and resid 58 and name N)	4.55	0.22	0.23
20	assign (segid 3A4 and resid 55 and name CA) (segid 3A4 and resid 58 and name O)	6.62	0.30	0.31
	assign (segid 3A4 and resid 55 and name CA) (segid 3A4 and resid 59 and name CA)	6.46	0.52	0.51
	assign (segid 3A4 and resid 55 and name CA) (segid 3A4 and resid 59 and name CB)	6.23	0.60	0.59
	assign (segid 3A4 and resid 55 and name CA) (segid 3A4 and resid 59 and name N)	5.48	0.59	0.60
	assign (segid 3A4 and resid 55 and name CA) (segid 3A4 and resid 68 and name CA)	16.28	2.31	2.30
25	assign (segid 3A4 and resid 55 and name CA) (segid 3A4 and resid 69 and name CA)	13.82	2.66	2.65
	assign (segid 3A4 and resid 55 and name CA) (segid 3A4 and resid 187 and name CB)	14.55	2.15	2.15
	assign (segid 3A4 and resid 55 and name CB) (segid 3A4 and resid 322 and name CA)	14.37	2.45	2.45
	assign (segid 3A4 and resid 55 and name CB) (segid 3A4 and resid 323 and name CA)	15.38	2.45	2.45
30	assign (segid 3A4 and resid 55 and name CB) (segid 3A4 and resid 324 and name CB)	14.84	2.60	2.60
	assign (segid 3A4 and resid 55 and name CB) (segid 3A4 and resid 324 and name CB)	13.92	2.62	2.62
	assign (segid 3A4 and resid 55 and name CB) (segid 3A4 and resid 342 and name CA)	13.46	3.07	3.08
	assign (segid 3A4 and resid 55 and name CB) (segid 3A4 and resid 56 and name C)	5.37	0.08	0.08
	assign (segid 3A4 and resid 55 and name CB) (segid 3A4 and resid 56 and name CA)	4.44	0.07	0.08
	assign (segid 3A4 and resid 55 and name CB) (segid 3A4 and resid 56 and name CB)	5.35	0.12	0.13
35	assign (segid 3A4 and resid 55 and name CB) (segid 3A4 and resid 56 and name N)	3.12	0.09	0.08
	assign (segid 3A4 and resid 55 and name CB) (segid 3A4 and resid 56 and name O)	6.12	0.20	0.20
	assign (segid 3A4 and resid 55 and name CB) (segid 3A4 and resid 57 and name C)	6.84	0.14	0.15
	assign (segid 3A4 and resid 55 and name CB) (segid 3A4 and resid 57 and name CA)	6.81	0.14	0.14
	assign (segid 3A4 and resid 55 and name CB) (segid 3A4 and resid 57 and name N)	5.64	0.15	0.16
40	assign (segid 3A4 and resid 55 and name CB) (segid 3A4 and resid 58 and name C)	6.70	0.14	0.14
	assign (segid 3A4 and resid 55 and name CB) (segid 3A4 and resid 58 and name CA)	6.34	0.12	0.13
	assign (segid 3A4 and resid 55 and name CB) (segid 3A4 and resid 58 and name N)	5.88	0.12	0.12
	assign (segid 3A4 and resid 55 and name CB) (segid 3A4 and resid 59 and name CA)	7.09	0.41	0.41
	assign (segid 3A4 and resid 55 and name CB) (segid 3A4 and resid 59 and name CB)	6.63	0.56	0.56
45	assign (segid 3A4 and resid 55 and name CB) (segid 3A4 and resid 59 and name N)	6.35	0.47	0.47
	assign (segid 3A4 and resid 55 and name CB) (segid 3A4 and resid 59 and name CA)	14.98	2.60	2.61
	assign (segid 3A4 and resid 55 and name N) (segid 3A4 and resid 55 and name C)	2.51	0.06	0.05
	assign (segid 3A4 and resid 55 and name N) (segid 3A4 and resid 55 and name CB)	1.46	0.01	0.00
50	assign (segid 3A4 and resid 55 and name N) (segid 3A4 and resid 55 and name CB)	2.45	0.02	0.02
	assign (segid 3A4 and resid 55 and name N) (segid 3A4 and resid 55 and name O)	3.50	0.04	0.05
	assign (segid 3A4 and resid 55 and name N) (segid 3A4 and resid 56 and name C)	4.88	0.15	0.14
	assign (segid 3A4 and resid 55 and name N) (segid 3A4 and resid 56 and name CA)	4.32	0.12	0.12
	assign (segid 3A4 and resid 55 and name N) (segid 3A4 and resid 56 and name CB)	4.99	0.13	0.12
	assign (segid 3A4 and resid 55 and name N) (segid 3A4 and resid 56 and name N)	2.91	0.11	0.11
55	assign (segid 3A4 and resid 55 and name N) (segid 3A4 and resid 56 and name O)	5.89	0.08	0.08
	assign (segid 3A4 and resid 55 and name N) (segid 3A4 and resid 57 and name C)	5.84	0.35	0.36
	assign (segid 3A4 and resid 55 and name N) (segid 3A4 and resid 57 and name CA)	5.57	0.30	0.31
	assign (segid 3A4 and resid 55 and name N) (segid 3A4 and resid 57 and name N)	4.56	0.30	0.30
60	assign (segid 3A4 and resid 55 and name N) (segid 3A4 and resid 57 and name O)	7.04	0.35	0.36
	assign (segid 3A4 and resid 55 and name N) (segid 3A4 and resid 58 and name C)	6.61	0.29	0.30
	assign (segid 3A4 and resid 55 and name N) (segid 3A4 and resid 58 and name CA)	5.78	0.40	0.40
	assign (segid 3A4 and resid 55 and name N) (segid 3A4 and resid 58 and name N)	5.01	0.39	0.39
	assign (segid 3A4 and resid 55 and name N) (segid 3A4 and resid 58 and name O)	7.56	0.15	0.16
	assign (segid 3A4 and resid 55 and name O) (segid 3A4 and resid 55 and name CB)	3.30	0.03	0.04
65	assign (segid 3A4 and resid 55 and name O) (segid 3A4 and resid 56 and name C)	2.84	0.09	0.10
	assign (segid 3A4 and resid 55 and name O) (segid 3A4 and resid 56 and name CA)	2.79	0.04	0.03
	assign (segid 3A4 and resid 55 and name O) (segid 3A4 and resid 56 and name CB)	4.24	0.05	0.04
	assign (segid 3A4 and resid 55 and name O) (segid 3A4 and resid 56 and name N)	2.25	0.02	0.01
70	assign (segid 3A4 and resid 55 and name O) (segid 3A4 and resid 56 and name O)	3.26	0.20	0.19
	assign (segid 3A4 and resid 55 and name O) (segid 3A4 and resid 57 and name C)	3.87	0.15	0.14
	assign (segid 3A4 and resid 55 and name O) (segid 3A4 and resid 57 and name CA)	4.14	0.14	0.14
	assign (segid 3A4 and resid 55 and name O) (segid 3A4 and resid 57 and name N)	3.25	0.11	0.11
	assign (segid 3A4 and resid 55 and name O) (segid 3A4 and resid 57 and name O)	4.85	0.16	0.16
75	assign (segid 3A4 and resid 55 and name O) (segid 3A4 and resid 58 and name C)	3.73	0.12	0.11
	assign (segid 3A4 and resid 55 and name O) (segid 3A4 and resid 58 and name CA)	3.56	0.11	0.12
	assign (segid 3A4 and resid 55 and name O) (segid 3A4 and resid 58 and name N)	3.02	0.16	0.15
	assign (segid 3A4 and resid 55 and name O) (segid 3A4 and resid 58 and name O)	4.70	0.33	0.34
	assign (segid 3A4 and resid 55 and name O) (segid 3A4 and resid 59 and name C)	5.39	0.62	0.61
80	assign (segid 3A4 and resid 55 and name O) (segid 3A4 and resid 59 and name CA)	4.16	0.53	0.53
	assign (segid 3A4 and resid 55 and name O) (segid 3A4 and resid 59 and name CB)	3.99	0.63	0.62
	assign (segid 3A4 and resid 55 and name O) (segid 3A4 and resid 59 and name N)	3.24	0.55	0.55
	assign (segid 3A4 and resid 55 and name O) (segid 3A4 and resid 59 and name O)	6.44	0.49	0.50

	assign (segid 3A4 and resid 56 and name C) (segid 3A4 and resid 56 and name CB)	2.48	0.03	0.03
	assign (segid 3A4 and resid 56 and name C) (segid 3A4 and resid 56 and name O)	1.23	0.00	0.01
	assign (segid 3A4 and resid 56 and name C) (segid 3A4 and resid 57 and name C)	3.04	0.04	0.04
	assign (segid 3A4 and resid 56 and name C) (segid 3A4 and resid 57 and name CA)	2.43	0.04	0.03
5	assign (segid 3A4 and resid 56 and name C) (segid 3A4 and resid 57 and name N)	1.32	0.00	0.01
	assign (segid 3A4 and resid 56 and name C) (segid 3A4 and resid 57 and name O)	3.96	0.08	0.07
	assign (segid 3A4 and resid 56 and name C) (segid 3A4 and resid 58 and name C)	4.53	0.19	0.19
	assign (segid 3A4 and resid 56 and name C) (segid 3A4 and resid 58 and name CA)	4.44	0.17	0.18
	assign (segid 3A4 and resid 56 and name C) (segid 3A4 and resid 58 and name N)	3.23	0.18	0.18
	assign (segid 3A4 and resid 56 and name C) (segid 3A4 and resid 58 and name O)	5.55	0.37	0.36
10	assign (segid 3A4 and resid 56 and name C) (segid 3A4 and resid 59 and name C)	5.13	0.42	0.42
	assign (segid 3A4 and resid 56 and name C) (segid 3A4 and resid 59 and name CA)	4.57	0.11	0.10
	assign (segid 3A4 and resid 56 and name C) (segid 3A4 and resid 59 and name CB)	4.27	0.14	0.14
	assign (segid 3A4 and resid 56 and name C) (segid 3A4 and resid 59 and name N)	3.87	0.11	0.11
	assign (segid 3A4 and resid 56 and name C) (segid 3A4 and resid 59 and name O)	6.29	0.33	0.33
15	assign (segid 3A4 and resid 56 and name CA) (segid 3A4 and resid 160 and name CA)	13.28	3.29	3.29
	assign (segid 3A4 and resid 56 and name CA) (segid 3A4 and resid 161 and name CA)	14.67	2.71	2.70
	assign (segid 3A4 and resid 56 and name CA) (segid 3A4 and resid 187 and name CA)	12.75	2.62	2.62
	assign (segid 3A4 and resid 56 and name CA) (segid 3A4 and resid 187 and name CB)	11.76	2.73	2.74
	assign (segid 3A4 and resid 56 and name CA) (segid 3A4 and resid 188 and name CA)	12.97	3.23	3.23
20	assign (segid 3A4 and resid 56 and name CA) (segid 3A4 and resid 324 and name CB)	16.01	2.08	2.08
	assign (segid 3A4 and resid 56 and name CA) (segid 3A4 and resid 56 and name C)	1.52	0.00	0.01
	assign (segid 3A4 and resid 56 and name CA) (segid 3A4 and resid 56 and name CB)	1.53	0.01	0.00
	assign (segid 3A4 and resid 56 and name CA) (segid 3A4 and resid 56 and name O)	2.41	0.02	0.01
	assign (segid 3A4 and resid 56 and name CA) (segid 3A4 and resid 57 and name C)	4.42	0.03	0.04
25	assign (segid 3A4 and resid 56 and name CA) (segid 3A4 and resid 57 and name CA)	3.78	0.04	0.05
	assign (segid 3A4 and resid 56 and name CA) (segid 3A4 and resid 57 and name N)	2.41	0.04	0.04
	assign (segid 3A4 and resid 56 and name CA) (segid 3A4 and resid 57 and name O)	5.41	0.09	0.09
	assign (segid 3A4 and resid 56 and name CA) (segid 3A4 and resid 58 and name C)	5.50	0.17	0.16
	assign (segid 3A4 and resid 56 and name CA) (segid 3A4 and resid 58 and name CA)	5.44	0.11	0.11
30	assign (segid 3A4 and resid 56 and name CA) (segid 3A4 and resid 58 and name N)	4.33	0.09	0.09
	assign (segid 3A4 and resid 56 and name CA) (segid 3A4 and resid 58 and name O)	6.50	0.44	0.43
	assign (segid 3A4 and resid 56 and name CA) (segid 3A4 and resid 59 and name C)	6.06	0.42	0.43
	assign (segid 3A4 and resid 56 and name CA) (segid 3A4 and resid 59 and name CA)	5.28	0.18	0.17
	assign (segid 3A4 and resid 56 and name CA) (segid 3A4 and resid 59 and name CB)	4.63	0.18	0.18
35	assign (segid 3A4 and resid 56 and name CA) (segid 3A4 and resid 59 and name N)	4.73	0.22	0.21
	assign (segid 3A4 and resid 56 and name CA) (segid 3A4 and resid 59 and name O)	7.17	0.30	0.30
	assign (segid 3A4 and resid 56 and name CA) (segid 3A4 and resid 69 and name CA)	14.16	2.68	2.68
	assign (segid 3A4 and resid 56 and name CB) (segid 3A4 and resid 160 and name CA)	12.96	3.48	3.48
40	assign (segid 3A4 and resid 56 and name CB) (segid 3A4 and resid 187 and name CA)	12.65	2.98	2.99
	assign (segid 3A4 and resid 56 and name CB) (segid 3A4 and resid 187 and name CB)	11.73	3.11	3.12
	assign (segid 3A4 and resid 56 and name CB) (segid 3A4 and resid 188 and name CA)	13.09	3.58	3.57
	assign (segid 3A4 and resid 56 and name CB) (segid 3A4 and resid 57 and name C)	5.36	0.07	0.08
	assign (segid 3A4 and resid 56 and name CB) (segid 3A4 and resid 57 and name CA)	4.36	0.10	0.10
	assign (segid 3A4 and resid 56 and name CB) (segid 3A4 and resid 57 and name N)	3.04	0.10	0.10
45	assign (segid 3A4 and resid 56 and name CB) (segid 3A4 and resid 57 and name O)	6.32	0.07	0.08
	assign (segid 3A4 and resid 56 and name CB) (segid 3A4 and resid 58 and name C)	6.88	0.16	0.16
	assign (segid 3A4 and resid 56 and name CB) (segid 3A4 and resid 58 and name CA)	6.75	0.10	0.10
	assign (segid 3A4 and resid 56 and name CB) (segid 3A4 and resid 58 and name N)	5.50	0.10	0.11
	assign (segid 3A4 and resid 56 and name CB) (segid 3A4 and resid 59 and name CA)	6.59	0.13	0.14
50	assign (segid 3A4 and resid 56 and name CB) (segid 3A4 and resid 59 and name CB)	5.85	0.09	0.10
	assign (segid 3A4 and resid 56 and name CB) (segid 3A4 and resid 59 and name N)	6.11	0.16	0.16
	assign (segid 3A4 and resid 56 and name N) (segid 3A4 and resid 56 and name C)	2.49	0.03	0.02
	assign (segid 3A4 and resid 56 and name N) (segid 3A4 and resid 56 and name CA)	1.46	0.01	0.01
	assign (segid 3A4 and resid 56 and name N) (segid 3A4 and resid 56 and name CB)	2.44	0.05	0.04
55	assign (segid 3A4 and resid 56 and name N) (segid 3A4 and resid 56 and name O)	3.48	0.05	0.05
	assign (segid 3A4 and resid 56 and name N) (segid 3A4 and resid 57 and name C)	4.74	0.13	0.14
	assign (segid 3A4 and resid 56 and name N) (segid 3A4 and resid 57 and name CA)	4.26	0.11	0.11
	assign (segid 3A4 and resid 56 and name N) (segid 3A4 and resid 57 and name N)	2.87	0.12	0.12
	assign (segid 3A4 and resid 56 and name N) (segid 3A4 and resid 57 and name O)	5.88	0.18	0.17
60	assign (segid 3A4 and resid 56 and name N) (segid 3A4 and resid 58 and name C)	5.62	0.07	0.08
	assign (segid 3A4 and resid 56 and name N) (segid 3A4 and resid 58 and name CA)	5.32	0.09	0.09
	assign (segid 3A4 and resid 56 and name N) (segid 3A4 and resid 58 and name N)	4.30	0.09	0.09
	assign (segid 3A4 and resid 56 and name N) (segid 3A4 and resid 58 and name O)	6.64	0.40	0.39
	assign (segid 3A4 and resid 56 and name N) (segid 3A4 and resid 59 and name CA)	5.80	0.32	0.32
65	assign (segid 3A4 and resid 56 and name N) (segid 3A4 and resid 59 and name CB)	5.27	0.36	0.36
	assign (segid 3A4 and resid 56 and name N) (segid 3A4 and resid 59 and name N)	5.04	0.39	0.38
	assign (segid 3A4 and resid 56 and name O) (segid 3A4 and resid 56 and name CB)	3.35	0.11	0.11
	assign (segid 3A4 and resid 56 and name O) (segid 3A4 and resid 57 and name C)	3.00	0.12	0.11
70	assign (segid 3A4 and resid 56 and name O) (segid 3A4 and resid 57 and name CA)	2.77	0.05	0.04
	assign (segid 3A4 and resid 56 and name O) (segid 3A4 and resid 57 and name N)	2.25	0.01	0.02
	assign (segid 3A4 and resid 56 and name O) (segid 3A4 and resid 57 and name O)	3.59	0.05	0.06
	assign (segid 3A4 and resid 56 and name O) (segid 3A4 and resid 58 and name C)	4.03	0.41	0.40
	assign (segid 3A4 and resid 56 and name O) (segid 3A4 and resid 58 and name CA)	4.30	0.40	0.40
	assign (segid 3A4 and resid 56 and name O) (segid 3A4 and resid 58 and name N)	3.33	0.38	0.37
75	assign (segid 3A4 and resid 56 and name O) (segid 3A4 and resid 58 and name O)	4.93	0.52	0.52
	assign (segid 3A4 and resid 56 and name O) (segid 3A4 and resid 59 and name C)	4.06	0.37	0.38
	assign (segid 3A4 and resid 56 and name O) (segid 3A4 and resid 59 and name CA)	3.70	0.12	0.12
	assign (segid 3A4 and resid 56 and name O) (segid 3A4 and resid 59 and name CB)	3.47	0.22	0.22
	assign (segid 3A4 and resid 56 and name O) (segid 3A4 and resid 59 and name N)	3.25	0.17	0.18
80	assign (segid 3A4 and resid 56 and name O) (segid 3A4 and resid 59 and name O)	5.19	0.29	0.30
	assign (segid 3A4 and resid 57 and name C) (segid 3A4 and resid 57 and name O)	1.23	0.00	0.01
	assign (segid 3A4 and resid 57 and name C) (segid 3A4 and resid 58 and name C)	3.05	0.10	0.10

	assign (segid 3A4 and resid 57 and name C) (segid 3A4 and resid 58 and name CA)	2.43	0.02	0.01
	assign (segid 3A4 and resid 57 and name C) (segid 3A4 and resid 58 and name N)	1.33	0.00	0.00
	assign (segid 3A4 and resid 57 and name C) (segid 3A4 and resid 58 and name O)	3.98	0.17	0.18
	assign (segid 3A4 and resid 57 and name C) (segid 3A4 and resid 59 and name C)	4.69	0.40	0.41
	assign (segid 3A4 and resid 57 and name C) (segid 3A4 and resid 59 and name CA)	4.40	0.11	0.11
5	assign (segid 3A4 and resid 57 and name C) (segid 3A4 and resid 59 and name CB)	5.04	0.16	0.16
	assign (segid 3A4 and resid 57 and name C) (segid 3A4 and resid 59 and name N)	3.20	0.07	0.08
	assign (segid 3A4 and resid 57 and name C) (segid 3A4 and resid 59 and name O)	5.79	0.42	0.41
	assign (segid 3A4 and resid 57 and name CA) (segid 3A4 and resid 157 and name CA)	15.43	2.20	2.20
	assign (segid 3A4 and resid 57 and name CA) (segid 3A4 and resid 158 and name CA)	15.84	2.34	2.33
10	assign (segid 3A4 and resid 57 and name CA) (segid 3A4 and resid 159 and name CA)	13.45	3.17	3.17
	assign (segid 3A4 and resid 57 and name CA) (segid 3A4 and resid 159 and name CB)	13.33	3.68	3.68
	assign (segid 3A4 and resid 57 and name CA) (segid 3A4 and resid 160 and name CA)	11.87	2.30	2.30
	assign (segid 3A4 and resid 57 and name CA) (segid 3A4 and resid 160 and name CB)	12.08	2.28	2.27
	assign (segid 3A4 and resid 57 and name CA) (segid 3A4 and resid 161 and name CA)	13.34	1.51	1.51
15	assign (segid 3A4 and resid 57 and name CA) (segid 3A4 and resid 161 and name CB)	14.30	1.42	1.42
	assign (segid 3A4 and resid 57 and name CA) (segid 3A4 and resid 187 and name CA)	11.66	2.96	2.97
	assign (segid 3A4 and resid 57 and name CA) (segid 3A4 and resid 187 and name CB)	10.70	3.08	3.08
	assign (segid 3A4 and resid 57 and name CA) (segid 3A4 and resid 188 and name CA)	12.06	3.31	3.32
	assign (segid 3A4 and resid 57 and name CA) (segid 3A4 and resid 189 and name CA)	14.93	3.49	3.49
20	assign (segid 3A4 and resid 57 and name CA) (segid 3A4 and resid 190 and name CA)	14.39	3.04	3.03
	assign (segid 3A4 and resid 57 and name CA) (segid 3A4 and resid 190 and name CB)	14.00	2.76	2.75
	assign (segid 3A4 and resid 57 and name CA) (segid 3A4 and resid 191 and name CA)	12.44	3.45	3.44
	assign (segid 3A4 and resid 57 and name CA) (segid 3A4 and resid 191 and name CB)	11.39	3.38	3.38
	assign (segid 3A4 and resid 57 and name CA) (segid 3A4 and resid 322 and name CA)	13.60	2.22	2.21
25	assign (segid 3A4 and resid 57 and name CA) (segid 3A4 and resid 323 and name CA)	15.29	2.15	2.14
	assign (segid 3A4 and resid 57 and name CA) (segid 3A4 and resid 324 and name CA)	16.01	1.92	1.93
	assign (segid 3A4 and resid 57 and name CA) (segid 3A4 and resid 324 and name CB)	15.17	1.85	1.85
	assign (segid 3A4 and resid 57 and name CA) (segid 3A4 and resid 431 and name CA)	13.69	2.36	2.36
	assign (segid 3A4 and resid 57 and name CA) (segid 3A4 and resid 57 and name C)	1.52	0.02	0.01
30	assign (segid 3A4 and resid 57 and name CA) (segid 3A4 and resid 57 and name O)	2.39	0.02	0.01
	assign (segid 3A4 and resid 57 and name CA) (segid 3A4 and resid 58 and name C)	4.41	0.07	0.07
	assign (segid 3A4 and resid 57 and name CA) (segid 3A4 and resid 58 and name CA)	3.80	0.02	0.03
	assign (segid 3A4 and resid 57 and name CA) (segid 3A4 and resid 58 and name N)	2.44	0.02	0.01
	assign (segid 3A4 and resid 57 and name CA) (segid 3A4 and resid 58 and name O)	5.38	0.11	0.10
35	assign (segid 3A4 and resid 57 and name CA) (segid 3A4 and resid 59 and name C)	5.61	0.47	0.46
	assign (segid 3A4 and resid 57 and name CA) (segid 3A4 and resid 59 and name CA)	5.34	0.13	0.14
	assign (segid 3A4 and resid 57 and name CA) (segid 3A4 and resid 59 and name CB)	5.64	0.20	0.19
	assign (segid 3A4 and resid 57 and name CA) (segid 3A4 and resid 59 and name N)	4.29	0.11	0.11
	assign (segid 3A4 and resid 57 and name CA) (segid 3A4 and resid 59 and name O)	6.74	0.46	0.46
40	assign (segid 3A4 and resid 57 and name CA) (segid 3A4 and resid 66 and name CA)	14.26	2.31	2.31
	assign (segid 3A4 and resid 57 and name CA) (segid 3A4 and resid 68 and name CA)	13.45	2.75	2.75
	assign (segid 3A4 and resid 57 and name CA) (segid 3A4 and resid 69 and name CA)	11.65	2.88	2.87
	assign (segid 3A4 and resid 57 and name CA) (segid 3A4 and resid 69 and name C)	2.46	0.04	0.03
	assign (segid 3A4 and resid 57 and name N) (segid 3A4 and resid 57 and name CA)	1.45	0.01	0.02
45	assign (segid 3A4 and resid 57 and name N) (segid 3A4 and resid 57 and name O)	3.53	0.05	0.05
	assign (segid 3A4 and resid 57 and name N) (segid 3A4 and resid 58 and name C)	4.70	0.04	0.03
	assign (segid 3A4 and resid 57 and name N) (segid 3A4 and resid 58 and name CA)	4.20	0.04	0.04
	assign (segid 3A4 and resid 57 and name N) (segid 3A4 and resid 58 and name N)	2.79	0.04	0.03
	assign (segid 3A4 and resid 57 and name N) (segid 3A4 and resid 58 and name O)	5.75	0.14	0.14
50	assign (segid 3A4 and resid 57 and name N) (segid 3A4 and resid 59 and name C)	5.82	0.46	0.46
	assign (segid 3A4 and resid 57 and name N) (segid 3A4 and resid 59 and name CA)	5.29	0.15	0.16
	assign (segid 3A4 and resid 57 and name N) (segid 3A4 and resid 59 and name CB)	5.25	0.16	0.17
	assign (segid 3A4 and resid 57 and name N) (segid 3A4 and resid 59 and name N)	4.32	0.18	0.18
	assign (segid 3A4 and resid 57 and name N) (segid 3A4 and resid 58 and name C)	3.07	0.21	0.21
55	assign (segid 3A4 and resid 57 and name O) (segid 3A4 and resid 58 and name CA)	2.75	0.03	0.03
	assign (segid 3A4 and resid 57 and name O) (segid 3A4 and resid 58 and name N)	2.25	0.01	0.01
	assign (segid 3A4 and resid 57 and name O) (segid 3A4 and resid 58 and name O)	3.73	0.42	0.42
	assign (segid 3A4 and resid 57 and name O) (segid 3A4 and resid 59 and name C)	4.31	0.47	0.47
60	assign (segid 3A4 and resid 57 and name O) (segid 3A4 and resid 59 and name CA)	4.36	0.16	0.16
	assign (segid 3A4 and resid 57 and name O) (segid 3A4 and resid 59 and name CB)	5.22	0.18	0.18
	assign (segid 3A4 and resid 57 and name O) (segid 3A4 and resid 59 and name N)	3.35	0.08	0.08
	assign (segid 3A4 and resid 57 and name O) (segid 3A4 and resid 59 and name O)	5.28	0.54	0.54
	assign (segid 3A4 and resid 58 and name C) (segid 3A4 and resid 58 and name O)	1.23	0.00	0.01
	assign (segid 3A4 and resid 58 and name C) (segid 3A4 and resid 59 and name C)	3.20	0.16	0.15
65	assign (segid 3A4 and resid 58 and name C) (segid 3A4 and resid 59 and name CA)	2.46	0.02	0.01
	assign (segid 3A4 and resid 58 and name C) (segid 3A4 and resid 59 and name CB)	3.67	0.08	0.08
	assign (segid 3A4 and resid 58 and name C) (segid 3A4 and resid 59 and name N)	1.34	0.01	0.00
	assign (segid 3A4 and resid 58 and name C) (segid 3A4 and resid 59 and name O)	4.02	0.16	0.16
	assign (segid 3A4 and resid 58 and name CA) (segid 3A4 and resid 160 and name CA)	13.70	2.36	2.36
70	assign (segid 3A4 and resid 58 and name CA) (segid 3A4 and resid 160 and name CB)	13.89	2.40	2.40
	assign (segid 3A4 and resid 58 and name CA) (segid 3A4 and resid 161 and name CA)	14.83	1.65	1.65
	assign (segid 3A4 and resid 58 and name CA) (segid 3A4 and resid 161 and name CB)	15.69	1.55	1.56
	assign (segid 3A4 and resid 58 and name CA) (segid 3A4 and resid 187 and name CA)	13.03	2.27	2.27
	assign (segid 3A4 and resid 58 and name CA) (segid 3A4 and resid 187 and name CB)	11.96	2.28	2.29
75	assign (segid 3A4 and resid 58 and name CA) (segid 3A4 and resid 188 and name CA)	12.88	2.63	2.63
	assign (segid 3A4 and resid 58 and name CA) (segid 3A4 and resid 189 and name CA)	16.18	2.75	2.75
	assign (segid 3A4 and resid 58 and name CA) (segid 3A4 and resid 190 and name CB)	15.62	2.42	2.42
	assign (segid 3A4 and resid 58 and name CA) (segid 3A4 and resid 191 and name CA)	13.50	3.01	3.01
	assign (segid 3A4 and resid 58 and name CA) (segid 3A4 and resid 191 and name CB)	12.20	2.96	2.97
80	assign (segid 3A4 and resid 58 and name CA) (segid 3A4 and resid 246 and name CA)	14.30	3.00	3.01
	assign (segid 3A4 and resid 58 and name CA) (segid 3A4 and resid 246 and name CB)	13.53	3.03	3.04
	assign (segid 3A4 and resid 58 and name CA) (segid 3A4 and resid 250 and name CA)	14.64	2.23	2.24

	assign	(segid 3A4 and resid 58 and name CA)	(segid 3A4 and resid 250 and name CB)	14.37	2.35	2.34
	assign	(segid 3A4 and resid 58 and name CA)	(segid 3A4 and resid 253 and name CA)	15.97	1.74	1.74
	assign	(segid 3A4 and resid 58 and name CA)	(segid 3A4 and resid 322 and name CA)	13.04	1.74	1.75
	assign	(segid 3A4 and resid 58 and name CA)	(segid 3A4 and resid 323 and name CA)	14.09	2.07	2.07
5	assign	(segid 3A4 and resid 58 and name CA)	(segid 3A4 and resid 323 and name CB)	15.54	2.09	2.08
	assign	(segid 3A4 and resid 58 and name CA)	(segid 3A4 and resid 324 and name CA)	14.28	2.09	2.08
	assign	(segid 3A4 and resid 58 and name CA)	(segid 3A4 and resid 324 and name CB)	13.26	2.05	2.06
	assign	(segid 3A4 and resid 58 and name CA)	(segid 3A4 and resid 326 and name CA)	18.66	1.70	1.69
	assign	(segid 3A4 and resid 58 and name CA)	(segid 3A4 and resid 340 and name CA)	16.27	2.00	2.00
10	assign	(segid 3A4 and resid 58 and name CA)	(segid 3A4 and resid 341 and name CA)	16.59	2.19	2.19
	assign	(segid 3A4 and resid 58 and name CA)	(segid 3A4 and resid 342 and name CA)	14.30	2.38	2.37
	assign	(segid 3A4 and resid 58 and name CA)	(segid 3A4 and resid 430 and name CA)	16.63	1.79	1.78
	assign	(segid 3A4 and resid 58 and name CA)	(segid 3A4 and resid 431 and name CA)	15.03	2.10	2.11
	assign	(segid 3A4 and resid 58 and name CA)	(segid 3A4 and resid 58 and name C)	1.53	0.00	0.00
15	assign	(segid 3A4 and resid 58 and name CA)	(segid 3A4 and resid 58 and name O)	2.41	0.01	0.01
	assign	(segid 3A4 and resid 58 and name CA)	(segid 3A4 and resid 59 and name C)	4.54	0.13	0.14
	assign	(segid 3A4 and resid 58 and name CA)	(segid 3A4 and resid 59 and name CA)	3.82	0.00	0.01
	assign	(segid 3A4 and resid 58 and name CA)	(segid 3A4 and resid 59 and name CB)	4.82	0.06	0.06
	assign	(segid 3A4 and resid 58 and name CA)	(segid 3A4 and resid 59 and name N)	2.44	0.01	0.00
20	assign	(segid 3A4 and resid 58 and name CA)	(segid 3A4 and resid 59 and name O)	5.46	0.16	0.15
	assign	(segid 3A4 and resid 58 and name CA)	(segid 3A4 and resid 66 and name CA)	13.43	1.96	1.96
	assign	(segid 3A4 and resid 58 and name CA)	(segid 3A4 and resid 67 and name CA)	15.16	1.92	1.92
	assign	(segid 3A4 and resid 58 and name CA)	(segid 3A4 and resid 67 and name CB)	16.44	1.96	1.95
	assign	(segid 3A4 and resid 58 and name CA)	(segid 3A4 and resid 68 and name CA)	12.96	1.75	1.75
25	assign	(segid 3A4 and resid 58 and name CA)	(segid 3A4 and resid 69 and name CA)	10.54	1.98	1.98
	assign	(segid 3A4 and resid 58 and name CA)	(segid 3A4 and resid 70 and name CA)	12.98	2.57	2.56
	assign	(segid 3A4 and resid 58 and name CA)	(segid 3A4 and resid 71 and name CA)	15.37	2.62	2.61
	assign	(segid 3A4 and resid 58 and name CA)	(segid 3A4 and resid 71 and name CB)	15.34	2.56	2.56
	assign	(segid 3A4 and resid 58 and name CA)	(segid 3A4 and resid 58 and name C)	2.44	0.03	0.02
30	assign	(segid 3A4 and resid 58 and name N)	(segid 3A4 and resid 58 and name CA)	1.46	0.01	0.01
	assign	(segid 3A4 and resid 58 and name N)	(segid 3A4 and resid 58 and name O)	3.48	0.08	0.08
	assign	(segid 3A4 and resid 58 and name N)	(segid 3A4 and resid 59 and name C)	4.83	0.26	0.26
	assign	(segid 3A4 and resid 58 and name N)	(segid 3A4 and resid 59 and name CA)	4.16	0.05	0.06
	assign	(segid 3A4 and resid 58 and name N)	(segid 3A4 and resid 59 and name CB)	4.83	0.11	0.11
35	assign	(segid 3A4 and resid 58 and name N)	(segid 3A4 and resid 59 and name N)	2.77	0.07	0.06
	assign	(segid 3A4 and resid 58 and name N)	(segid 3A4 and resid 59 and name O)	5.91	0.24	0.23
	assign	(segid 3A4 and resid 58 and name O)	(segid 3A4 and resid 59 and name C)	3.26	0.25	0.25
	assign	(segid 3A4 and resid 58 and name O)	(segid 3A4 and resid 59 and name CA)	2.80	0.04	0.03
40	assign	(segid 3A4 and resid 58 and name O)	(segid 3A4 and resid 59 and name CB)	4.19	0.13	0.12
	assign	(segid 3A4 and resid 58 and name O)	(segid 3A4 and resid 59 and name N)	2.25	0.01	0.02
	assign	(segid 3A4 and resid 59 and name C)	(segid 3A4 and resid 59 and name O)	3.74	0.27	0.26
45	assign	(segid 3A4 and resid 59 and name C)	(segid 3A4 and resid 59 and name CB)	2.50	0.02	0.01
	assign	(segid 3A4 and resid 59 and name CA)	(segid 3A4 and resid 59 and name O)	1.24	0.01	0.00
	assign	(segid 3A4 and resid 59 and name CA)	(segid 3A4 and resid 160 and name CA)	14.30	2.77	2.76
	assign	(segid 3A4 and resid 59 and name CA)	(segid 3A4 and resid 160 and name CB)	14.47	2.58	2.58
50	assign	(segid 3A4 and resid 59 and name CA)	(segid 3A4 and resid 161 and name CA)	15.63	2.28	2.28
	assign	(segid 3A4 and resid 59 and name CA)	(segid 3A4 and resid 161 and name CB)	16.47	2.29	2.30
	assign	(segid 3A4 and resid 59 and name CA)	(segid 3A4 and resid 187 and name CA)	12.50	2.08	2.08
	assign	(segid 3A4 and resid 59 and name CA)				

5	assign (segid HEM and resid 1 and name C2A) (segid HEM and resid 1 and name C2A) (segid HEM and resid 1 and name CMA) 2.58 0.03 0.03
	assign (segid HEM and resid 1 and name C2A) (segid HEM and resid 1 and name CMB) 6.60 0.02 0.03
	assign (segid HEM and resid 1 and name C2A) (segid HEM and resid 1 and name CMD) 7.52 0.04 0.03
	assign (segid HEM and resid 1 and name C2A) (segid HEM and resid 1 and name C1A) 4.35 0.06 0.07
	assign (segid HEM and resid 1 and name C2A) (segid HEM and resid 1 and name C2A) 4.75 0.14 0.14
	assign (segid HEM and resid 1 and name C2A) (segid HEM and resid 1 and name C2D) 6.82 0.19 0.18
	assign (segid HEM and resid 1 and name C2B) (segid HEM and resid 1 and name C1C) 4.74 0.03 0.03
	assign (segid HEM and resid 1 and name C2B) (segid HEM and resid 1 and name C1D) 7.28 0.05 0.06
	assign (segid HEM and resid 1 and name C2B) (segid HEM and resid 1 and name C2C) 6.07 0.03 0.03
	assign (segid HEM and resid 1 and name C2B) (segid HEM and resid 1 and name C3B) 1.36 0.02 0.02
10	assign (segid HEM and resid 1 and name C2B) (segid HEM and resid 1 and name C3C) 6.95 0.03 0.03
	assign (segid HEM and resid 1 and name C2B) (segid HEM and resid 1 and name C4B) 2.26 0.02 0.02
	assign (segid HEM and resid 1 and name C2B) (segid HEM and resid 1 and name C4C) 6.39 0.03 0.03
	assign (segid HEM and resid 1 and name C2B) (segid HEM and resid 1 and name C4D) 7.08 0.05 0.04
15	assign (segid HEM and resid 1 and name C2B) (segid HEM and resid 1 and name CAB) 2.53 0.04 0.04
	assign (segid HEM and resid 1 and name C2B) (segid HEM and resid 1 and name CBB) 3.23 0.05 0.06
	assign (segid HEM and resid 1 and name C2B) (segid HEM and resid 1 and name CMB) 1.53 0.01 0.01
	assign (segid HEM and resid 1 and name C2B) (segid HEM and resid 1 and name CMC) 6.65 0.05 0.05
20	assign (segid HEM and resid 1 and name C2C) (segid HEM and resid 1 and name C1D) 4.69 0.04 0.04
	assign (segid HEM and resid 1 and name C2C) (segid HEM and resid 1 and name C2D) 6.03 0.04 0.03
	assign (segid HEM and resid 1 and name C2C) (segid HEM and resid 1 and name C3C) 1.37 0.02 0.02
	assign (segid HEM and resid 1 and name C2C) (segid HEM and resid 1 and name C3D) 6.90 0.04 0.04
	assign (segid HEM and resid 1 and name C2C) (segid HEM and resid 1 and name C4C) 2.25 0.01 0.01
	assign (segid HEM and resid 1 and name C2C) (segid HEM and resid 1 and name C4D) 6.35 0.02 0.02
25	assign (segid HEM and resid 1 and name C2C) (segid HEM and resid 1 and name CAC) 2.54 0.05 0.04
	assign (segid HEM and resid 1 and name C2C) (segid HEM and resid 1 and name CBC) 3.28 0.06 0.07
	assign (segid HEM and resid 1 and name C2C) (segid HEM and resid 1 and name CMC) 1.54 0.02 0.01
	assign (segid HEM and resid 1 and name C2C) (segid HEM and resid 1 and name CMD) 6.64 0.02 0.02
	assign (segid HEM and resid 1 and name C2D) (segid HEM and resid 1 and name C3D) 1.35 0.02 0.01
30	assign (segid HEM and resid 1 and name C2D) (segid HEM and resid 1 and name C4D) 2.25 0.01 0.01
	assign (segid HEM and resid 1 and name C2D) (segid HEM and resid 1 and name CAD) 2.58 0.03 0.03
	assign (segid HEM and resid 1 and name C2D) (segid HEM and resid 1 and name CBD) 3.46 0.05 0.05
	assign (segid HEM and resid 1 and name C2D) (segid HEM and resid 1 and name CGD) 4.85 0.06 0.07
	assign (segid HEM and resid 1 and name C2D) (segid HEM and resid 1 and name CMD) 1.53 0.01 0.01
35	assign (segid HEM and resid 1 and name C2D) (segid HEM and resid 1 and name C1D) 5.57 0.14 0.15
	assign (segid HEM and resid 1 and name C2D) (segid HEM and resid 1 and name C2D) 5.44 0.14 0.14
	assign (segid HEM and resid 1 and name C3A) (segid HEM and resid 1 and name C1B) 3.78 0.02 0.02
	assign (segid HEM and resid 1 and name C3A) (segid HEM and resid 1 and name C1C) 7.04 0.02 0.03
	assign (segid HEM and resid 1 and name C3A) (segid HEM and resid 1 and name C1D) 6.36 0.03 0.04
40	assign (segid HEM and resid 1 and name C3A) (segid HEM and resid 1 and name C2B) 4.99 0.02 0.01
	assign (segid HEM and resid 1 and name C3A) (segid HEM and resid 1 and name C2D) 6.93 0.04 0.05
	assign (segid HEM and resid 1 and name C3A) (segid HEM and resid 1 and name C3B) 6.01 0.02 0.02
	assign (segid HEM and resid 1 and name C3A) (segid HEM and resid 1 and name C3D) 6.06 0.05 0.05
	assign (segid HEM and resid 1 and name C3A) (segid HEM and resid 1 and name C4A) 1.44 0.02 0.03
45	assign (segid HEM and resid 1 and name C3A) (segid HEM and resid 1 and name C4B) 5.70 0.02 0.01
	assign (segid HEM and resid 1 and name C3A) (segid HEM and resid 1 and name C4C) 7.25 0.03 0.04
	assign (segid HEM and resid 1 and name C3A) (segid HEM and resid 1 and name C4D) 4.71 0.04 0.05
	assign (segid HEM and resid 1 and name C3A) (segid HEM and resid 1 and name CAA) 2.56 0.05 0.06
	assign (segid HEM and resid 1 and name C3A) (segid HEM and resid 1 and name CAB) 7.41 0.06 0.05
50	assign (segid HEM and resid 1 and name C3A) (segid HEM and resid 1 and name CAD) 6.67 0.06 0.06
	assign (segid HEM and resid 1 and name C3A) (segid HEM and resid 1 and name CBA) 3.36 0.04 0.05
	assign (segid HEM and resid 1 and name C3A) (segid HEM and resid 1 and name CBD) 7.16 0.10 0.09
	assign (segid HEM and resid 1 and name C3A) (segid HEM and resid 1 and name CGA) 4.71 0.05 0.04
	assign (segid HEM and resid 1 and name C3A) (segid HEM and resid 1 and name CMA) 1.53 0.01 0.00
55	assign (segid HEM and resid 1 and name C3A) (segid HEM and resid 1 and name CMB) 5.38 0.03 0.03
	assign (segid HEM and resid 1 and name C3A) (segid HEM and resid 1 and name C1A) 5.19 0.12 0.11
	assign (segid HEM and resid 1 and name C3A) (segid HEM and resid 1 and name C2A) 5.54 0.10 0.09
	assign (segid HEM and resid 1 and name C3B) (segid HEM and resid 1 and name C1C) 3.82 0.02 0.02
60	assign (segid HEM and resid 1 and name C3B) (segid HEM and resid 1 and name C1D) 7.06 0.06 0.05
	assign (segid HEM and resid 1 and name C3B) (segid HEM and resid 1 and name C2C) 5.03 0.03 0.02
	assign (segid HEM and resid 1 and name C3B) (segid HEM and resid 1 and name C3C) 6.06 0.02 0.02
	assign (segid HEM and resid 1 and name C3B) (segid HEM and resid 1 and name C4B) 1.45 0.01 0.02
	assign (segid HEM and resid 1 and name C3B) (segid HEM and resid 1 and name C4C) 5.74 0.02 0.02
	assign (segid HEM and resid 1 and name C3B) (segid HEM and resid 1 and name C4D)

	assign	(segid HEM and resid	1 and name CHB)	(segid HEM and resid	1 and name C2D)	7.32	0.05	0.04
	assign	(segid HEM and resid	1 and name CHB)	(segid HEM and resid	1 and name C3A)	2.49	0.01	0.01
	assign	(segid HEM and resid	1 and name CHB)	(segid HEM and resid	1 and name C3B)	3.57	0.03	0.02
	assign	(segid HEM and resid	1 and name CHB)	(segid HEM and resid	1 and name C3C)	7.31	0.03	0.03
5	assign	(segid HEM and resid	1 and name CHB)	(segid HEM and resid	1 and name C3D)	6.86	0.05	0.05
	assign	(segid HEM and resid	1 and name CHB)	(segid HEM and resid	1 and name C4A)	1.38	0.01	0.02
	assign	(segid HEM and resid	1 and name CHB)	(segid HEM and resid	1 and name C4B)	3.51	0.02	0.03
	assign	(segid HEM and resid	1 and name CHB)	(segid HEM and resid	1 and name C4C)	6.30	0.03	0.03
	assign	(segid HEM and resid	1 and name CHB)	(segid HEM and resid	1 and name C4D)	5.41	0.04	0.05
10	assign	(segid HEM and resid	1 and name CHB)	(segid HEM and resid	1 and name CAA)	4.99	0.05	0.05
	assign	(segid HEM and resid	1 and name CHB)	(segid HEM and resid	1 and name CAB)	4.94	0.06	0.06
	assign	(segid HEM and resid	1 and name CHB)	(segid HEM and resid	1 and name CAD)	7.89	0.05	0.05
	assign	(segid HEM and resid	1 and name CHB)	(segid HEM and resid	1 and name CBA)	5.72	0.05	0.05
	assign	(segid HEM and resid	1 and name CHB)	(segid HEM and resid	1 and name CBB)	5.73	0.06	0.06
15	assign	(segid HEM and resid	1 and name CHB)	(segid HEM and resid	1 and name CGA)	7.12	0.06	0.05
	assign	(segid HEM and resid	1 and name CHB)	(segid HEM and resid	1 and name CHC)	4.80	0.03	0.03
	assign	(segid HEM and resid	1 and name CHB)	(segid HEM and resid	1 and name CHD)	6.81	0.04	0.03
	assign	(segid HEM and resid	1 and name CHB)	(segid HEM and resid	1 and name CMA)	3.12	0.04	0.05
	assign	(segid HEM and resid	1 and name CHB)	(segid HEM and resid	1 and name CMB)	3.12	0.03	0.02
20	assign	(segid HEM and resid	1 and name CHB)	(segid HEM and resid	1 and name CMC)	7.87	0.04	0.04
	assign	(segid HEM and resid	1 and name CHB)	(segid HEM and resid	1 and name OLA)	7.63	0.11	0.11
	assign	(segid HEM and resid	1 and name CHC)	(segid HEM and resid	1 and name C1A)	6.27	0.03	0.02
	assign	(segid HEM and resid	1 and name CHC)	(segid HEM and resid	1 and name C1B)	3.52	0.02	0.03
	assign	(segid HEM and resid	1 and name CHC)	(segid HEM and resid	1 and name C1C)	1.39	0.01	0.01
25	assign	(segid HEM and resid	1 and name CHC)	(segid HEM and resid	1 and name C1D)	5.37	0.05	0.05
	assign	(segid HEM and resid	1 and name CHC)	(segid HEM and resid	1 and name C2A)	7.26	0.03	0.03
	assign	(segid HEM and resid	1 and name CHC)	(segid HEM and resid	1 and name C2B)	3.60	0.03	0.02
	assign	(segid HEM and resid	1 and name CHC)	(segid HEM and resid	1 and name C2C)	2.51	0.02	0.02
	assign	(segid HEM and resid	1 and name CHC)	(segid HEM and resid	1 and name C2D)	6.82	0.06	0.05
30	assign	(segid HEM and resid	1 and name CHC)	(segid HEM and resid	1 and name C3A)	6.81	0.02	0.02
	assign	(segid HEM and resid	1 and name CHC)	(segid HEM and resid	1 and name C3B)	2.52	0.01	0.01
	assign	(segid HEM and resid	1 and name CHC)	(segid HEM and resid	1 and name C3C)	3.58	0.01	0.02
	assign	(segid HEM and resid	1 and name CHC)	(segid HEM and resid	1 and name C3D)	7.27	0.05	0.05
	assign	(segid HEM and resid	1 and name CHC)	(segid HEM and resid	1 and name C4A)	5.37	0.03	0.02
35	assign	(segid HEM and resid	1 and name CHC)	(segid HEM and resid	1 and name C4B)	1.39	0.01	0.01
	assign	(segid HEM and resid	1 and name CHC)	(segid HEM and resid	1 and name C4C)	3.51	0.01	0.02
	assign	(segid HEM and resid	1 and name CHC)	(segid HEM and resid	1 and name C4D)	6.26	0.04	0.05
	assign	(segid HEM and resid	1 and name CHC)	(segid HEM and resid	1 and name CAB)	3.01	0.03	0.03
40	assign	(segid HEM and resid	1 and name CHC)	(segid HEM and resid	1 and name CAC)	4.95	0.04	0.05
	assign	(segid HEM and resid	1 and name CHC)	(segid HEM and resid	1 and name CBB)	4.32	0.07	0.06
	assign	(segid HEM and resid	1 and name CHC)	(segid HEM and resid	1 and name CBC)	5.75	0.06	0.06
	assign	(segid HEM and resid	1 and name CHC)	(segid HEM and resid	1 and name CHD)	4.79	0.03	0.04
	assign	(segid HEM and resid	1 and name CHC)	(segid HEM and resid	1 and name CMA)	7.86	0.04	0.03
45	assign	(segid HEM and resid	1 and name CHC)	(segid HEM and resid	1 and name CMB)	5.06	0.02	0.02
	assign	(segid HEM and resid	1 and name CHC)	(segid HEM and resid	1 and name CMC)	3.13	0.04	0.04
	assign	(segid HEM and resid	1 and name CHD)	(segid HEM and resid	1 and name CMD)	7.86	0.04	0.04
	assign	(segid HEM and resid	1 and name CHD)	(segid HEM and resid	1 and name CIA)	5.40	0.04	0.03
50	assign	(segid HEM and resid	1 and name CHD)	(segid HEM and resid	1 and name C1B)	6.31	0.03	0.03
	assign	(segid HEM and resid	1 and name CHD)	(segid HEM and resid	1 and name C1C)	3.51	0.03	0.03
	assign	(segid HEM and resid	1 and name CHD)	(segid HEM and resid	1 and name C1D)	1.38	0.02	0.01
	assign	(segid HEM and resid	1 and name CHD)	(segid HEM and resid	1 and name C2A)	6.83	0.03	0.03
	assign	(segid HEM and resid	1 and name CHD)	(segid HEM and resid	1 and name C2B)	7.32	0.03	0.03
	assign	(segid HEM and resid	1 and name CHD)	(segid HEM and resid	1 and name C2C)	3.58	0.03	0.02
55	assign	(segid HEM and resid	1 and name CHD)	(segid HEM and resid	1 and name C2D)	2.50	0.03	0.02
	assign	(segid HEM and resid	1 and name CHD)	(segid HEM and resid	1 and name C3A)	7.29	0.03	0.04
	assign	(segid HEM and resid	1 and name CHD)	(segid HEM and resid	1 and name C3B)	6.85	0.03	0.03
	assign	(segid HEM and resid	1 and name CHD)	(segid HEM and resid	1 and name C3C)	2.49	0.03	0.03
	assign	(segid HEM and resid	1 and name CHD)	(segid HEM and resid	1 and name C3D)	3.56	0.02	0.02
60	assign	(segid HEM and resid	1 and name CHD)	(segid HEM and resid	1 and name C4A)	6.29	0.04	0.04
	assign	(segid HEM and resid	1 and name CHD)	(segid HEM and resid	1 and name C4B)	5.40	0.04	0.04
	assign	(segid HEM and resid	1 and name CHD)	(segid HEM and resid	1 and name C4C)	1.38	0.02	0.02
	assign	(segid HEM and resid	1 and name CHD)	(segid HEM and resid	1 and name C4D)	3.51	0.02	0.03
	assign	(segid HEM and resid	1 and name CHD)	(segid HEM and resid	1 and name CAA)	7.89	0.05	0.04
65	assign	(segid HEM and resid	1 and name CHD)	(segid HEM and resid	1 and name CAB)	7.73	0.06	0.07
	assign	(segid HEM and resid	1 and name CHD)	(segid HEM and resid	1 and name CAC)	2.99	0.06	0.06
	assign	(segid HEM and resid	1 and name CHD)	(segid HEM and resid	1 and name CAD)	5.01	0.03	0.03
	assign	(segid HEM and resid	1 and name CHD)	(segid HEM and resid	1 and name CBC)	4.13	0.17	0.17
	assign	(segid HEM and resid	1 and name CHD)	(segid HEM and resid	1 and name CBD)	5.77	0.08	0.07
	assign	(segid HEM and resid	1 and name CHD)	(segid HEM and resid	1 and name CBD)	7.24	0.08	0.08
70	assign	(segid HEM and resid	1 and name CHD)	(segid HEM and resid	1 and name CMC)	5.04	0.03	0.03
	assign	(segid HEM and resid	1 and name CHD)	(segid HEM and resid	1 and name CMD)	3.13	0.02	0.03
	assign	(segid HEM and resid	1 and name CMA)	(segid HEM and resid	1 and name C1B)	4.50	0.04	0.05
	assign	(segid HEM and resid	1 and name CMA)	(segid HEM and resid	1 and name C1D)	7.88	0.04	0.05
	assign	(segid HEM and resid	1 and name CMA)	(segid HEM and resid	1 and name C2B)	5.42	0.03	0.03
75	assign	(segid HEM and resid	1 and name CMA)	(segid HEM and resid	1 and name C3B)	6.63	0.04	0.04
	assign	(segid HEM and resid	1 and name CMA)	(segid HEM and resid	1 and name C3D)	7.52	0.05	0.05
	assign	(segid HEM and resid	1 and name CMA)	(segid HEM and resid	1 and name C4B)	6.62	0.03	0.03
	assign	(segid HEM and resid	1 and name CMA)	(segid HEM and resid	1 and name C4D)	6.21	0.05	0.05
	assign	(segid HEM and resid	1 and name CMA)	(segid HEM and resid	1 and name CAA)	3.17	0.10	0.10
80	assign	(segid HEM and resid	1 and name CMA)	(segid HEM and resid	1 and name CAB)	7.94	0.04	0.03
	assign	(segid HEM and resid	1 and name CMA)	(segid HEM and resid	1 and name CBA)	3.74	0.15	0.16
	assign	(segid HEM and resid	1 and name CMA)	(segid HEM and resid	1 and name CGA)	4.85	0.05	0.05
	assign	(segid HEM and resid	1 and name CMA)	(segid HEM and resid	1 and name CMB)	5.38	0.05	0.05

	assign	(segid HEM and resid	1 and name CMA)	(segid HEM and resid	1 and name O1A)	5.24	0.21	0.21
	assign	(segid HEM and resid	1 and name CMA)	(segid HEM and resid	1 and name O2A)	5.63	0.12	0.12
	assign	(segid HEM and resid	1 and name CMB)	(segid HEM and resid	1 and name C1C)	6.25	0.03	0.03
	assign	(segid HEM and resid	1 and name CMB)	(segid HEM and resid	1 and name C2C)	7.55	0.02	0.03
5	assign	(segid HEM and resid	1 and name CMB)	(segid HEM and resid	1 and name C4C)	7.91	0.02	0.03
	assign	(segid HEM and resid	1 and name CMB)	(segid HEM and resid	1 and name CAB)	3.26	0.04	0.05
	assign	(segid HEM and resid	1 and name CMC)	(segid HEM and resid	1 and name CBB)	3.37	0.08	0.07
	assign	(segid HEM and resid	1 and name CMC)	(segid HEM and resid	1 and name C1D)	6.20	0.04	0.04
10	assign	(segid HEM and resid	1 and name CMC)	(segid HEM and resid	1 and name C2D)	7.51	0.03	0.04
	assign	(segid HEM and resid	1 and name CMC)	(segid HEM and resid	1 and name C4D)	7.87	0.03	0.03
	assign	(segid HEM and resid	1 and name CMD)	(segid HEM and resid	1 and name CAC)	3.27	0.06	0.05
	assign	(segid HEM and resid	1 and name CMD)	(segid HEM and resid	1 and name CBC)	3.52	0.14	0.14
	assign	(segid HEM and resid	1 and name CMD)	(segid HEM and resid	1 and name CAD)	3.20	0.06	0.06
	assign	(segid HEM and resid	1 and name CMD)	(segid HEM and resid	1 and name CBD)	3.93	0.09	0.08
15	assign	(segid HEM and resid	1 and name CMD)	(segid HEM and resid	1 and name CGD)	5.09	0.08	0.09
	assign	(segid HEM and resid	1 and name CMD)	(segid HEM and resid	1 and name O1D)	5.66	0.18	0.18
	assign	(segid HEM and resid	1 and name FE)	(segid HEM and resid	1 and name O2D)	5.71	0.12	0.11
	assign	(segid HEM and resid	1 and name FE)	(segid HEM and resid	1 and name C1A)	3.04	0.01	0.02
	assign	(segid HEM and resid	1 and name FE)	(segid HEM and resid	1 and name C1B)	3.05	0.02	0.03
20	assign	(segid HEM and resid	1 and name FE)	(segid HEM and resid	1 and name C1C)	3.02	0.03	0.03
	assign	(segid HEM and resid	1 and name FE)	(segid HEM and resid	1 and name C1D)	3.05	0.03	0.03
	assign	(segid HEM and resid	1 and name FE)	(segid HEM and resid	1 and name C2A)	4.27	0.02	0.02
	assign	(segid HEM and resid	1 and name FE)	(segid HEM and resid	1 and name C2B)	4.29	0.03	0.03
	assign	(segid HEM and resid	1 and name FE)	(segid HEM and resid	1 and name C2C)	4.26	0.02	0.03
25	assign	(segid HEM and resid	1 and name FE)	(segid HEM and resid	1 and name C2D)	4.29	0.03	0.02
	assign	(segid HEM and resid	1 and name FE)	(segid HEM and resid	1 and name C3A)	4.28	0.03	0.02
	assign	(segid HEM and resid	1 and name FE)	(segid HEM and resid	1 and name C3B)	4.26	0.03	0.04
	assign	(segid HEM and resid	1 and name FE)	(segid HEM and resid	1 and name C3C)	4.27	0.04	0.04
	assign	(segid HEM and resid	1 and name FE)	(segid HEM and resid	1 and name C3D)	4.28	0.03	0.03
30	assign	(segid HEM and resid	1 and name FE)	(segid HEM and resid	1 and name C4A)	3.04	0.01	0.02
	assign	(segid HEM and resid	1 and name FE)	(segid HEM and resid	1 and name C4B)	3.02	0.03	0.04
	assign	(segid HEM and resid	1 and name FE)	(segid HEM and resid	1 and name C4C)	3.04	0.04	0.05
	assign	(segid HEM and resid	1 and name FE)	(segid HEM and resid	1 and name C4D)	3.04	0.01	0.02
	assign	(segid HEM and resid	1 and name FE)	(segid HEM and resid	1 and name CAA)	5.66	0.02	0.02
35	assign	(segid HEM and resid	1 and name FE)	(segid HEM and resid	1 and name CAB)	5.51	0.07	0.07
	assign	(segid HEM and resid	1 and name FE)	(segid HEM and resid	1 and name CAC)	5.53	0.07	0.08
	assign	(segid HEM and resid	1 and name FE)	(segid HEM and resid	1 and name CAD)	5.67	0.02	0.02
	assign	(segid HEM and resid	1 and name FE)	(segid HEM and resid	1 and name CBA)	6.41	0.19	0.19
	assign	(segid HEM and resid	1 and name FE)	(segid HEM and resid	1 and name CBB)	6.75	0.07	0.07
40	assign	(segid HEM and resid	1 and name FE)	(segid HEM and resid	1 and name CBC)	6.65	0.11	0.12
	assign	(segid HEM and resid	1 and name FE)	(segid HEM and resid	1 and name CBD)	6.33	0.03	0.04
	assign	(segid HEM and resid	1 and name FE)	(segid HEM and resid	1 and name CGA)	7.80	0.10	0.10
	assign	(segid HEM and resid	1 and name FE)	(segid HEM and resid	1 and name CGD)	7.77	0.07	0.06
	assign	(segid HEM and resid	1 and name FE)	(segid HEM and resid	1 and name CHA)	3.41	0.02	0.02
45	assign	(segid HEM and resid	1 and name FE)	(segid HEM and resid	1 and name CHB)	3.43	0.04	0.04
	assign	(segid HEM and resid	1 and name FE)	(segid HEM and resid	1 and name CHC)	3.37	0.03	0.03
	assign	(segid HEM and resid	1 and name FE)	(segid HEM and resid	1 and name CHD)	3.42	0.05	0.04
	assign	(segid HEM and resid	1 and name NA)	(segid HEM and resid	1 and name CMA)	5.68	0.04	0.04
50	assign	(segid						

627

	assign (segid HEM and resid 1 and name ND) (segid HEM and resid 1 and name C2D) 2.33 0.03 0.03
	assign (segid HEM and resid 1 and name ND) (segid HEM and resid 1 and name C3A) 5.01 0.05 0.04
	assign (segid HEM and resid 1 and name ND) (segid HEM and resid 1 and name C3B) 6.25 0.07 0.07
	assign (segid HEM and resid 1 and name ND) (segid HEM and resid 1 and name C3C) 4.39 0.02 0.03
5	assign (segid HEM and resid 1 and name ND) (segid HEM and resid 1 and name C3D) 2.32 0.03 0.03
	assign (segid HEM and resid 1 and name ND) (segid HEM and resid 1 and name C4A) 4.20 0.05 0.04
	assign (segid HEM and resid 1 and name ND) (segid HEM and resid 1 and name C4B) 4.94 0.07 0.07
	assign (segid HEM and resid 1 and name ND) (segid HEM and resid 1 and name C4C) 2.96 0.03 0.03
	assign (segid HEM and resid 1 and name ND) (segid HEM and resid 1 and name C4D) 1.38 0.02 0.02
10	assign (segid HEM and resid 1 and name ND) (segid HEM and resid 1 and name CAA) 5.47 0.04 0.04
	assign (segid HEM and resid 1 and name ND) (segid HEM and resid 1 and name CAB) 7.45 0.10 0.10
	assign (segid HEM and resid 1 and name ND) (segid HEM and resid 1 and name CAC) 5.29 0.07 0.07
	assign (segid HEM and resid 1 and name ND) (segid HEM and resid 1 and name CAD) 3.79 0.02 0.02
	assign (segid HEM and resid 1 and name ND) (segid HEM and resid 1 and name CBA) 6.10 0.25 0.26
15	assign (segid HEM and resid 1 and name ND) (segid HEM and resid 1 and name CBC) 6.42 0.15 0.16
	assign (segid HEM and resid 1 and name ND) (segid HEM and resid 1 and name CBD) 4.57 0.05 0.06
	assign (segid HEM and resid 1 and name ND) (segid HEM and resid 1 and name CGA) 7.33 0.08 0.09
	assign (segid HEM and resid 1 and name ND) (segid HEM and resid 1 and name CGD) 6.03 0.05 0.06
	assign (segid HEM and resid 1 and name ND) (segid HEM and resid 1 and name CHA) 2.45 0.02 0.02
20	assign (segid HEM and resid 1 and name ND) (segid HEM and resid 1 and name CHB) 5.03 0.05 0.05
	assign (segid HEM and resid 1 and name ND) (segid HEM and resid 1 and name CHC) 4.99 0.06 0.05
	assign (segid HEM and resid 1 and name ND) (segid HEM and resid 1 and name CHD) 2.43 0.01 0.01
	assign (segid HEM and resid 1 and name ND) (segid HEM and resid 1 and name CMA) 6.52 0.05 0.06
	assign (segid HEM and resid 1 and name ND) (segid HEM and resid 1 and name CMB) 7.61 0.05 0.05
25	assign (segid HEM and resid 1 and name ND) (segid HEM and resid 1 and name CMC) 6.50 0.04 0.04
	assign (segid HEM and resid 1 and name ND) (segid HEM and resid 1 and name CMD) 3.79 0.02 0.03
	assign (segid HEM and resid 1 and name ND) (segid HEM and resid 1 and name O1D) 6.82 0.16 0.15
	assign (segid HEM and resid 1 and name ND) (segid HEM and resid 1 and name O2D) 6.54 0.16 0.15
	assign (segid HEM and resid 1 and name ND) (segid HEM and resid 1 and name C3D) 7.27 0.27 0.27
30	assign (segid HEM and resid 1 and name O1A) (segid HEM and resid 1 and name C4D) 6.73 0.19 0.20
	assign (segid HEM and resid 1 and name O1A) (segid HEM and resid 1 and name CAD) 6.72 0.34 0.34
	assign (segid HEM and resid 1 and name O1A) (segid HEM and resid 1 and name CBD) 6.69 0.43 0.42
	assign (segid HEM and resid 1 and name O1A) (segid HEM and resid 1 and name CGD) 6.52 0.45 0.46
	assign (segid HEM and resid 1 and name O1A) (segid HEM and resid 1 and name O2A) 2.17 0.05 0.05
35	assign (segid HEM and resid 1 and name O1A) (segid HEM and resid 1 and name O2D) 6.20 0.51 0.50
	assign (segid HEM and resid 1 and name O1D) (segid HEM and resid 1 and name O2D) 2.17 0.04 0.04
	assign (segid HEM and resid 1 and name O2A) (segid HEM and resid 1 and name C3D) 7.34 0.31 0.31
	assign (segid HEM and resid 1 and name O2A) (segid HEM and resid 1 and name C4D) 6.86 0.24 0.24
	assign (segid HEM and resid 1 and name O2A) (segid HEM and resid 1 and name CAD) 6.80 0.39 0.40
40	assign (segid HEM and resid 1 and name O2A) (segid HEM and resid 1 and name CBD) 6.91 0.38 0.39
	assign (segid HEM and resid 1 and name O2A) (segid HEM and resid 1 and name CGD) 6.75 0.44 0.45
	assign (segid HEM and resid 1 and name O2A) (segid HEM and resid 1 and name O2D) 6.46 0.53 0.53
	assign (segid HEM and resid 1 and name O2A) (segid HEM and resid 246 and name C) 6.08 0.73 0.73
	assign (segid 3A4 and resid 66 and name C) (segid 3A4 and resid 246 and name CB) 6.16 0.52 0.53
45	assign (segid 3A4 and resid 66 and name C) (segid 3A4 and resid 246 and name O) 5.92 0.84 0.85
	assign (segid 3A4 and resid 66 and name C) (segid 3A4 and resid 247 and name CA) 5.79 0.80 0.79
	assign (segid 3A4 and resid 66 and name C) (segid 3A4 and resid 247 and name CB) 6.07 0.82 0.82
	assign (segid 3A4 and resid 66 and name C) (segid 3A4 and resid 247 and name N) 5.99 0.70 0.71
	assign (segid 3A4 and resid 66 and name C) (segid 3A4 and resid 250 and name CB) 5.75 0.67 0.68
50	assign (segid 3A4 and resid 66 and name C) (segid HEM and resid 1 and name CGD) 7.00 0.44 0.45
	assign (segid 3A4 and resid 66 and name C) (segid HEM and resid 1 and name O1D) 7.08 0.55 0.55
	assign (segid 3A4 and resid 66 and name C) (segid HEM and resid 1 and name O2D) 6.82 0.50 0.50
	assign (segid 3A4 and resid 66 and name C) (segid 3A4 and resid 66 and name O) 1.23 0.00 0.01
	assign (segid 3A4 and resid 66 and name C) (segid 3A4 and resid 67 and name C) 3.16 0.12 0.13
	assign (segid 3A4 and resid 66 and name C) (segid 3A4 and resid 67 and name CA) 2.44 0.02 0.02
55	assign (segid 3A4 and resid 66 and name C) (segid 3A4 and resid 67 and name CB) 3.66 0.05 0.05
	assign (segid 3A4 and resid 66 and name C) (segid 3A4 and resid 67 and name N) 1.32 0.01 0.01
	assign (segid 3A4 and resid 66 and name C) (segid 3A4 and resid 67 and name O) 4.10 0.17 0.17
	assign (segid 3A4 and resid 66 and name C) (segid 3A4 and resid 68 and name C) 5.01 0.27 0.27
	assign (segid 3A4 and resid 66 and name C) (segid 3A4 and resid 68 and name CA) 4.64 0.27 0.27
60	assign (segid 3A4 and resid 66 and name C) (segid 3A4 and resid 68 and name N) 3.35 0.28 0.28
	assign (segid 3A4 and resid 66 and name C) (segid 3A4 and resid 68 and name O) 5.94 0.42 0.43
	assign (segid 3A4 and resid 66 and name C) (segid 3A4 and resid 69 and name C) 5.59 0.64 0.63
	assign (segid 3A4 and resid 66 and name C) (segid 3A4 and resid 69 and name CA) 5.54 0.70 0.69
	assign (segid 3A4 and resid 66 and name C) (segid 3A4 and resid 69 and name N) 4.62 0.71 0.71
65	assign (segid 3A4 and resid 66 and name C) (segid 3A4 and resid 70 and name CA) 6.03 0.69 0.69
	assign (segid 3A4 and resid 66 and name C) (segid 3A4 and resid 70 and name N) 5.44 0.78 0.78
	assign (segid 3A4 and resid 66 and name C) (segid 3A4 and resid 70 and name O) 7.09 0.41 0.40
	assign (segid 3A4 and resid 66 and name C) (segid 3A4 and resid 75 and name CA) 6.71 0.62 0.63
	assign (segid 3A4 and resid 66 and name C) (segid 3A4 and resid 75 and name CG) 7.14 0.27 0.27
70	assign (segid 3A4 and resid 66 and name C) (segid 3A4 and resid 78 and name CA) 6.83 0.69 0.69
	assign (segid 3A4 and resid 66 and name C) (segid 3A4 and resid 78 and name CB) 5.48 0.67 0.67
	assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 134 and name CA) 17.33 0.53 0.54
	assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 135 and name CA) 18.98 0.41 0.42
75	assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 137 and name CA) 16.97 1.55 1.55
	assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 138 and name CA) 16.25 0.53 0.53
	assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 138 and name CB) 15.70 0.85 0.86
	assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 157 and name CA) 17.62 1.31 1.31
	assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 160 and name CA) 17.30 1.11 1.11
80	assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 160 and name CB) 16.54 1.23 1.23
	assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 188 and name CA) 17.89 1.08 1.09
	assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 191 and name CA) 14.76 0.94 0.94
	assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 191 and name CB) 14.18 1.05 1.05

assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 192 and name CA) 16.40 0.59 0.60
 assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 192 and name CB) 17.56 0.59 0.59
 assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 193 and name CA) 18.10 0.65 0.65
 assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 194 and name CA) 15.13 0.78 0.78
 assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 194 and name CB) 14.20 0.88 0.88
 5 assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 195 and name CA) 13.58 0.49 0.49
 assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 195 and name CB) 13.32 0.44 0.44
 assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 196 and name CA) 17.00 0.46 0.47
 assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 196 and name CB) 18.28 0.45 0.45
 assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 197 and name CA) 15.61 0.57 0.57
 10 assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 197 and name CB) 17.49 0.69 0.68
 assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 198 and name CA) 14.43 0.60 0.60
 assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 198 and name CB) 12.96 0.61 0.61
 assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 199 and name CA) 15.31 0.56 0.56
 assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 199 and name CB) 15.61 0.58 0.58
 15 assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 200 and name CA) 18.76 0.58 0.57
 assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 201 and name CA) 17.81 0.56 0.57
 assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 201 and name CB) 17.06 0.62 0.62
 assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 202 and name CA) 15.83 0.59 0.60
 assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 202 and name CB) 14.60 0.65 0.66
 20 assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 205 and name CB) 18.33 0.62 0.61
 assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 219 and name CA) 18.30 0.65 0.65
 assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 219 and name CB) 18.42 0.66 0.65
 assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 220 and name CA) 14.66 0.67 0.66
 assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 220 and name CB) 13.78 0.73 0.73
 25 assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 221 and name CA) 14.15 0.55 0.54
 assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 221 and name CB) 14.65 0.56 0.55
 assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 222 and name CA) 17.06 0.56 0.56
 assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 222 and name CB) 18.44 0.54 0.54
 30 assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 223 and name CA) 15.91 0.56 0.56
 assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 223 and name CB) 15.70 0.59 0.59
 assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 224 and name CA) 12.66 0.61 0.61
 assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 224 and name CB) 11.51 0.58 0.58
 assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 225 and name CA) 14.82 0.83 0.83
 35 assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 225 and name CB) 15.74 0.84 0.85
 assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 226 and name CA) 17.36 0.88 0.88
 assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 240 and name CA) 11.62 0.61 0.61
 assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 240 and name CB) 11.46 0.62 0.63
 assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 241 and name CA) 12.04 0.54 0.53
 40 assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 241 and name CB) 13.33 0.54 0.55
 assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 242 and name CA) 9.69 0.62 0.61
 assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 242 and name CB) 10.02 0.60 0.60
 assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 243 and name CA) 6.70 0.64 0.63
 assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 243 and name CB) 6.92 0.62 0.63
 45 assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 243 and name O) 5.75 0.73 0.72
 assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 244 and name CA) 8.38 0.73 0.74
 assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 244 and name CB) 9.88 0.73 0.72
 assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 245 and name CA) 8.85 0.66 0.67
 assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 245 and name CB) 9.68 0.66 0.65
 50 assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 246 and name C) 4.95 0.61 0.61
 assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 246 and name CA) 5.54 0.57 0.58
 assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 246 and name CB) 4.77 0.53 0.53
 assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 246 and name O) 4.92 0.67 0.66
 assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 247 and name C) 6.38 0.53 0.52
 55 assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 247 and name CA) 5.09 0.55 0.55
 assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 247 and name CB) 5.54 0.60 0.59
 assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 247 and name N) 4.99 0.56 0.57
 assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 247 and name O) 6.63 0.49 0.50
 assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 248 and name CA) 8.69 0.54 0.53
 60 assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 248 and name CB) 9.75 0.56 0.57
 assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 249 and name CA) 8.61 0.55 0.56
 assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 250 and name CA) 6.84 0.53 0.54
 assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 250 and name CB) 5.52 0.52 0.53
 assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 251 and name CA) 9.33 0.39 0.39
 65 assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 251 and name CB) 9.62 0.40 0.41
 assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 252 and name CA) 12.01 0.43 0.44
 assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 252 and name CB) 12.24 0.47 0.47
 assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 253 and name CA) 11.85 0.55 0.55
 assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 254 and name CA) 11.40 0.55 0.55
 70 assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 255 and name CA) 13.92 0.51 0.52
 assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 256 and name CA) 16.48 0.47 0.46
 assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 257 and name CA) 17.64 0.63 0.63
 assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 258 and name CA) 17.86 0.71 0.71
 assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 258 and name CB) 16.78 0.77 0.76
 75 assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 319 and name CB) 17.14 1.01 1.01
 assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 322 and name CA) 15.79 0.62 0.61
 assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 323 and name CA) 15.97 0.88 0.88
 assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 323 and name CB) 16.66 1.00 1.01
 80 assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 324 and name CA) 17.45 0.91 0.90
 assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 324 and name CB) 16.81 0.91 0.91
 assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 384 and name CA) 17.59 0.65 0.64
 assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 384 and name CB) 17.81 0.57 0.58
 assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 385 and name CA) 16.98 0.87 0.87

	assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 386 and name CA)	17.99	0.75	0.74
	assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 387 and name CA)	16.99	0.60	0.60
	assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 388 and name CA)	14.15	0.69	0.70
	assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 388 and name CB)	13.95	0.84	0.84
5	assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 389 and name CA)	11.73	0.68	0.69
	assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 389 and name CB)	11.41	0.86	0.87
	assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 390 and name CA)	14.20	0.54	0.53
	assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 390 and name CB)	15.42	0.54	0.53
	assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 391 and name CA)	13.30	0.50	0.49
10	assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 391 and name CB)	14.29	0.52	0.51
	assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 392 and name CA)	12.40	0.32	0.31
	assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 392 and name CB)	11.06	0.31	0.32
	assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 393 and name CA)	14.27	0.56	0.57
	assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 394 and name CA)	17.32	0.45	0.45
	assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 394 and name CB)	17.60	0.40	0.41
15	assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 396 and name CB)	17.77	0.68	0.68
	assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 397 and name CB)	18.68	0.51	0.50
	assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 66 and name C)	1.53	0.01	0.01
	assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 66 and name O)	2.39	0.02	0.02
20	assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 67 and name C)	4.38	0.33	0.33
	assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 67 and name CA)	3.67	0.26	0.26
	assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 67 and name CB)	4.75	0.15	0.16
	assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 67 and name N)	2.44	0.01	0.01
	assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 67 and name O)	5.34	0.30	0.30
25	assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 68 and name C)	5.84	0.22	0.21
	assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 68 and name CA)	5.59	0.35	0.35
	assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 68 and name N)	4.38	0.36	0.37
	assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 68 and name O)	6.73	0.49	0.49
	assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 69 and name C)	6.17	0.26	0.27
30	assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 69 and name CA)	6.08	0.50	0.51
	assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 69 and name N)	5.33	0.65	0.65
	assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 69 and name O)	6.58	0.56	0.55
	assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 70 and name CA)	6.77	0.31	0.30
	assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 70 and name N)	6.20	0.50	0.50
35	assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 71 and name CA)	10.05	0.39	0.39
	assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 71 and name CB)	11.12	0.50	0.50
	assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 72 and name CA)	11.69	0.73	0.72
	assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 73 and name CA)	12.24	1.01	1.02
	assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 73 and name CB)	13.29	1.27	1.26
40	assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 74 and name CA)	8.96	1.13	1.14
	assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 74 and name CB)	8.30	1.26	1.27
	assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 75 and name C)	7.69	0.60	0.60
	assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 75 and name CB)	8.23	0.48	0.48
	assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 76 and name CA)	10.72	0.54	0.55
45	assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 76 and name CB)	12.08	0.58	0.59
	assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 77 and name CA)	10.52	0.70	0.69
	assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 77 and name CB)	10.73	0.73	0.73
	assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 78 and name CA)	7.36	0.69	0.68
	assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 78 and name CB)	5.94	0.69	0.70
50	assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 79 and name CA)	8.71	0.51	0.52
	assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 79 and name CB)	9.12	0.43	0.44
	assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 80 and name CA)	12.05	0.55	0.56
	assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 81 and name CA)	11.54	0.69	0.68
	assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 81 and name CB)	10.74	0.65	0.65
55	assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 82 and name CA)	10.77	1.02	1.01
	assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 82 and name CB)	9.58	1.06	1.06
	assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 83 and name CA)	13.19	0.53	0.53
	assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 83 and name CB)	13.48	0.48	0.48
	assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 84 and name CA)	16.00	1.03	1.03
60	assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 84 and name CB)	16.33	1.28	1.29
	assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 85 and name CA)	15.71	1.11	1.11
	assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 85 and name CB)	14.89	1.13	1.14
	assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 86 and name CA)	15.27	0.93	0.92
	assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 86 and name CB)	14.07	0.86	0.86
65	assign (segid 3A4 and resid 66 and name CA) (segid 3A4 and resid 246 and name C)	5.26	0.77	0.77
	assign (segid 3A4 and resid 66 and name N) (segid 3A4 and resid 246 and name CA)	5.54	0.71	0.70
	assign (segid 3A4 and resid 66 and name N) (segid 3A4 and resid 246 and name CB)	4.54	0.65	0.65
	assign (segid 3A4 and resid 66 and name N) (segid 3A4 and resid 246 and name O)	5.25	0.92	0.92
	assign (segid 3A4 and resid 66 and name N) (segid 3A4 and resid 247 and name CA)	5.88	0.71	0.71
70	assign (segid 3A4 and resid 66 and name N) (segid 3A4 and resid 247 and name CB)	6.43	0.70	0.70
	assign (segid 3A4 and resid 66 and name N) (segid 3A4 and resid 247 and name N)	5.51	0.70	0.71
	assign (segid 3A4 and resid 66 and name N) (segid 3A4 and resid 250 and name CB)	6.19	0.71	0.71
	assign (segid 3A4 and resid 66 and name N) (segid 3A4 and resid 66 and name C)	2.40	0.03	0.03
	assign (segid 3A4 and resid 66 and name N) (segid 3A4 and resid 66 and name CA)	1.45	0.00	0.00
75	assign (segid 3A4 and resid 66 and name N) (segid 3A4 and resid 66 and name O)	2.62	0.07	0.07
	assign (segid 3A4 and resid 66 and name N) (segid 3A4 and resid 67 and name C)	5.18	0.30	0.31
	assign (segid 3A4 and resid 66 and name N) (segid 3A4 and resid 67 and name CA)	4.71	0.20	0.20
	assign (segid 3A4 and resid 66 and name N) (segid 3A4 and resid 67 and name CB)	5.96	0.13	0.13
	assign (segid 3A4 and resid 66 and name N) (segid 3A4 and resid 67 and name N)	3.60	0.04	0.04
80	assign (segid 3A4 and resid 66 and name N) (segid 3A4 and resid 67 and name O)	6.00	0.20	0.20
	assign (segid 3A4 and resid 66 and name N) (segid 3A4 and resid 68 and name C)	6.06	0.32	0.32
	assign (segid 3A4 and resid 66 and name N) (segid 3A4 and resid 68 and name CA)	6.10	0.50	0.51
	assign (segid 3A4 and resid 66 and name N) (segid 3A4 and resid 68 and name N)	5.10	0.49	0.50

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assign (segid 3A4 and resid 66 and name N ) (segid 3A4 and resid 68 and name O ) 6.90 0.31 0.31
assign (segid 3A4 and resid 66 and name N ) (segid 3A4 and resid 69 and name C ) 5.88 0.47 0.17
assign (segid 3A4 and resid 66 and name N ) (segid 3A4 and resid 69 and name CA ) 5.83 0.69 0.70
assign (segid 3A4 and resid 66 and name N ) (segid 3A4 and resid 69 and name N ) 5.36 0.81 0.80
assign (segid 3A4 and resid 66 and name N ) (segid 3A4 and resid 69 and name O ) 6.13 0.66 0.67
5 assign (segid 3A4 and resid 66 and name N ) (segid 3A4 and resid 70 and name CA ) 6.63 0.48 0.47
assign (segid 3A4 and resid 66 and name N ) (segid 3A4 and resid 70 and name N ) 6.08 0.56 0.56
assign (segid 3A4 and resid 66 and name N ) (segid 3A4 and resid 78 and name CB ) 6.80 0.83 0.83
assign (segid 3A4 and resid 66 and name N ) (segid 3A4 and resid 250 and name CB ) 6.35 1.04 1.05
10 assign (segid 3A4 and resid 66 and name O ) (segid 3A4 and resid 1 and name CGD) 7.11 0.30 0.31
assign (segid 3A4 and resid 66 and name O ) (segid HEM and resid 1 and name O1D) 7.16 0.52 0.52
assign (segid 3A4 and resid 66 and name O ) (segid HEM and resid 1 and name O2D) 6.86 0.31 0.32
assign (segid 3A4 and resid 66 and name O ) (segid HEM and resid 67 and name C ) 3.27 0.50 0.49
assign (segid 3A4 and resid 66 and name O ) (segid 3A4 and resid 67 and name CA ) 2.90 0.26 0.26
15 assign (segid 3A4 and resid 66 and name O ) (segid 3A4 and resid 67 and name CB ) 4.25 0.12 0.12
assign (segid 3A4 and resid 66 and name O ) (segid 3A4 and resid 67 and name N ) 2.24 0.01 0.01
assign (segid 3A4 and resid 66 and name O ) (segid 3A4 and resid 67 and name O ) 3.96 0.65 0.65
assign (segid 3A4 and resid 66 and name O ) (segid 3A4 and resid 68 and name C ) 4.71 0.84 0.83
assign (segid 3A4 and resid 66 and name O ) (segid 3A4 and resid 68 and name CA ) 4.58 0.62 0.62
20 assign (segid 3A4 and resid 66 and name O ) (segid 3A4 and resid 68 and name N ) 3.49 0.57 0.56
assign (segid 3A4 and resid 66 and name O ) (segid 3A4 and resid 68 and name O ) 5.64 0.78 0.77
assign (segid 3A4 and resid 66 and name O ) (segid 3A4 and resid 69 and name CA ) 4.97 1.33 1.33
assign (segid 3A4 and resid 66 and name O ) (segid 3A4 and resid 69 and name N ) 4.17 1.25 1.25
assign (segid 3A4 and resid 66 and name O ) (segid 3A4 and resid 70 and name N ) 4.81 1.41 1.42
25 assign (segid 3A4 and resid 66 and name O ) (segid 3A4 and resid 78 and name CB ) 5.90 0.95 0.95
assign (segid 3A4 and resid 67 and name C ) (segid 3A4 and resid 250 and name CB ) 6.78 0.82 0.82
assign (segid 3A4 and resid 67 and name C ) (segid HEM and resid 1 and name C2D) 6.88 0.69 0.68
assign (segid 3A4 and resid 67 and name C ) (segid HEM and resid 1 and name C3D) 6.41 0.59 0.60
30 assign (segid 3A4 and resid 67 and name C ) (segid HEM and resid 1 and name CAD) 5.11 0.50 0.51
assign (segid 3A4 and resid 67 and name C ) (segid HEM and resid 1 and name CBD) 5.26 0.40 0.40
assign (segid 3A4 and resid 67 and name C ) (segid HEM and resid 1 and name CGD) 4.41 0.27 0.26
assign (segid 3A4 and resid 67 and name C ) (segid HEM and resid 1 and name CMD) 6.37 0.79 0.78
35 assign (segid 3A4 and resid 67 and name C ) (segid HEM and resid 1 and name O1D) 4.51 0.55 0.56
assign (segid 3A4 and resid 67 and name C ) (segid HEM and resid 1 and name O2D) 4.08 0.28 0.29
assign (segid 3A4 and resid 67 and name C ) (segid 3A4 and resid 67 and name CB ) 2.50 0.03 0.02
40 assign (segid 3A4 and resid 67 and name C ) (segid 3A4 and resid 67 and name O ) 1.24 0.02 0.01
assign (segid 3A4 and resid 67 and name C ) (segid 3A4 and resid 68 and name C ) 3.15 0.05 0.06
assign (segid 3A4 and resid 67 and name C ) (segid 3A4 and resid 68 and name CA ) 2.43 0.01 0.01
45 assign (segid 3A4 and resid 67 and name C ) (segid 3A4 and resid 68 and name N ) 1.33 0.00 0.01
assign (segid 3A4 and resid 67 and name C ) (segid 3A4 and resid 68 and name O ) 4.06 0.20 0.19
50 assign (segid 3A4 and resid 67 and name C ) (segid 3A4 and resid 69 and name C ) 4.81 0.18 0.21
assign (segid 3A4 and resid 67 and name C ) (segid 3A4 and resid 69 and name N ) 4.65 0.22 0.22
55 assign (segid 3A4 and resid 67 and name C ) (segid 3A4 and resid 69 and name O ) 5.70 0.45 0.44
assign (segid 3A4 and resid 67 and name C ) (segid 3A4 and resid 70 and name C ) 5.64 0.58 0.57
assign (segid 3A4 and resid 67 and name C ) (segid 3A4 and resid 70 and name CA ) 5.12 0.62 0.61
60 assign (segid 3A4 and resid 67 and name C ) (segid 3A4 and resid 70 and name N ) 4.35 0.64 0.64
assign (segid 3A4 and resid 67 and name C ) (segid 3A4 and resid 70 and name O ) 5.24 0.65 0.65
assign (segid 3A4 and resid 67 and name C ) (segid 3A4 and resid 75 and name C ) 6.56 0.38 0.38
65 assign (segid 3A4 and resid 67 and name C ) (segid 3A4 and resid 75 and name CA ) 5.81 0.30 0.31
assign (segid 3A4 and resid 67 and name C ) (segid 3A4 and resid 75 and name CB ) 5.67 0.28 0.28
assign (segid 3A4 and resid 67 and name C ) (segid 3A4 and resid 75 and name CG ) 5.19 0.33 0.34
70 assign (segid 3A4 and resid 67 and name C ) (segid 3A4 and resid 75 and name N ) 6.82 0.28 0.29
assign (segid 3A4 and resid 67 and name C ) (segid 3A4 and resid 75 and name O ) 6.30 0.42 0.43
75 assign (segid 3A4 and resid 67 and name C ) (segid 3A4 and resid 78 and name CB ) 6.39 0.39 0.38
assign (segid 3A4 and resid 67 and name C ) (segid 3A4 and resid 79 and name CB ) 6.84 0.43 0.44
assign (segid 3A4 and resid 67 and name C ) (segid 3A4 and resid 79 and name N ) 6.87 0.41 0.42
80 assign (segid 3A4 and resid 67 and name CA ) (segid 3A4 and resid 134 and name CA ) 17.78 0.53 0.53
assign (segid 3A4 and resid 67 and name CA ) (segid 3A4 and resid 137 and name CA ) 17.29 1.59 1.60
assign (segid 3A4 and resid 67 and name CA ) (segid 3A4 and resid 138 and name CA ) 17.20 0.41 0.42
assign (segid 3A4 and resid 67 and name CA ) (segid 3A4 and resid 138 and name CB ) 16.86 0.65 0.64
assign (segid 3A4 and resid 67 and name CA ) (segid 3A4 and resid 191 and name CA ) 17.63 1.11 1.11
assign (segid 3A4 and resid 67 and name CA ) (segid 3A4 and resid 191 and name CB ) 17.08 1.17 1.17
assign (segid 3A4 and resid 67 and name CA ) (segid 3A4 and resid 194 and name CA ) 17.90 0.99 0.99
75 assign (segid 3A4 and resid 67 and name CA ) (segid 3A4 and resid 194 and name CB ) 16.87 1.08 1.08
assign (segid 3A4 and resid 67 and name CA ) (segid 3A4 and resid 195 and name CA ) 16.73 0.72 0.72
assign (segid 3A4 and resid 67 and name CA ) (segid 3A4 and resid 195 and name CB ) 16.58 0.69 0.69
80 assign (segid 3A4 and resid 67 and name CA ) (segid 3A4 and resid 198 and name CA ) 17.11 0.69 0.69
assign (segid 3A4 and resid 67 and name CA ) (segid 3A4 and resid 198 and name CB ) 15.67 0.71 0.70
assign (segid 3A4 and resid 67 and name CA ) (segid 3A4 and resid 199 and name CA ) 18.29 0.58 0.57
assign (segid 3A4 and resid 67 and name CA ) (segid 3A4 and resid 199 and name CB ) 18.74 0.62 0.62
assign (segid 3A4 and resid 67 and name CA ) (segid 3A4 and resid 202 and name CA ) 18.18 0.46 0.45
assign (segid 3A4 and resid 67 and name CA ) (segid 3A4 and resid 202 and name CB ) 17.09 0.52 0.52
75 assign (segid 3A4 and resid 67 and name CA ) (segid 3A4 and resid 219 and name CA ) 18.66 0.87 0.88
assign (segid 3A4 and resid 67 and name CA ) (segid 3A4 and resid 220 and name CA ) 14.95 0.85 0.85
assign (segid 3A4 and resid 67 and name CA ) (segid 3A4 and resid 220 and name CB ) 13.99 0.93 0.92
80 assign (segid 3A4 and resid 67 and name CA ) (segid 3A4 and resid 221 and name CA ) 15.31 0.55 0.54
assign (segid 3A4 and resid 67 and name CA ) (segid 3A4 and resid 221 and name CB ) 16.05 0.54 0.55
assign (segid 3A4 and resid 67 and name CA ) (segid 3A4 and resid 222 and name CA ) 18.02 0.52 0.52
assign (segid 3A4 and resid 67 and name CA ) (segid 3A4 and resid 223 and name CA ) 16.22 0.59 0.58
assign (segid 3A4 and resid 67 and name CA ) (segid 3A4 and resid 223 and name CB ) 15.72 0.70 0.70
assign (segid 3A4 and resid 67 and name CA ) (segid 3A4 and resid 224 and name CA ) 13.41 0.55 0.54
assign (segid 3A4 and resid 67 and name CA ) (segid 3A4 and resid 224 and name CB ) 12.45 0.54 0.53

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	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 225 and name CA)	16.19	0.73	0.72
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 225 and name CB)	17.24	0.72	0.72
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 226 and name CA)	18.19	0.76	0.76
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 240 and name CA)	13.90	0.35	0.34
5	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 240 and name CB)	13.87	0.38	0.38
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 241 and name CA)	14.80	0.36	0.36
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 241 and name CB)	16.19	0.38	0.39
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 242 and name CA)	12.89	0.52	0.52
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 242 and name CB)	13.26	0.57	0.56
10	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 243 and name CA)	9.51	0.45	0.45
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 243 and name CB)	9.34	0.41	0.41
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 244 and name CA)	10.73	0.59	0.60
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 244 and name CB)	12.14	0.58	0.58
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 245 and name CA)	11.80	0.69	0.69
15	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 245 and name CB)	12.83	0.67	0.68
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 246 and name CA)	8.76	0.63	0.63
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 246 and name CB)	8.21	0.51	0.51
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 247 and name CA)	6.99	0.70	0.69
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 247 and name CB)	7.03	0.63	0.64
20	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 248 and name CA)	10.46	0.76	0.77
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 248 and name CB)	11.74	0.74	0.75
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 249 and name CA)	10.79	0.83	0.84
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 250 and name CA)	8.04	0.85	0.84
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 250 and name CB)	6.55	0.84	0.84
25	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 251 and name CA)	9.62	0.82	0.83
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 251 and name CB)	9.92	0.78	0.78
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 252 and name CA)	12.92	0.83	0.83
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 252 and name CB)	13.53	0.83	0.83
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 253 and name CA)	12.71	0.89	0.88
30	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 254 and name CA)	11.17	0.78	0.78
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 255 and name CA)	13.53	0.99	0.99
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 256 and name CA)	16.55	0.89	0.88
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 257 and name CA)	17.60	0.90	0.91
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 258 and name CA)	17.07	0.90	0.89
35	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 258 and name CB)	15.79	0.91	0.90
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 319 and name CA)	16.96	0.71	0.71
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 319 and name CB)	15.62	0.71	0.71
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 322 and name CA)	14.34	0.42	0.42
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 323 and name CA)	14.27	0.64	0.64
40	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 323 and name CB)	14.69	0.74	0.74
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 324 and name CA)	16.11	0.69	0.69
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 324 and name CB)	15.74	0.68	0.67
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 326 and name CB)	17.54	1.00	1.00
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 344 and name CA)	18.71	0.31	0.32
45	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 344 and name CB)	19.52	0.26	0.26
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 345 and name CA)	18.64	0.73	0.72
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 345 and name CB)	17.69	0.87	0.87
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 347 and name CB)	18.43	0.93	0.93
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 382 and name CA)	18.98	0.54	0.54
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 382 and name CB)	18.95	0.60	0.60
50	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 382 and name CB)	18.19	0.59	0.58
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 383 and name CA)	14.95	0.50	0.50
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 384 and name CA)	15.10	0.48	0.48
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 384 and name CB)	14.11	0.61	0.62
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 385 and name CA)	14.74	0.55	0.54
55	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 386 and name CA)	13.53	0.43	0.44
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 387 and name CA)	10.62	0.63	0.64
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 388 and name CA)	10.49	0.84	0.84
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 389 and name CA)	8.37	0.54	0.55
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 389 and name CB)	8.25	0.70	0.70
60	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 390 and name CA)	10.93	0.42	0.42
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 390 and name CB)	12.07	0.41	0.41
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 391 and name CA)	10.51	0.49	0.50
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 391 and name CB)	11.69	0.52	0.52
65	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 392 and name CA)	9.72	0.59	0.60
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 392 and name CB)	8.49	0.65	0.66
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 393 and name CA)	12.26	0.79	0.78
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 394 and name CA)	14.91	0.65	0.64
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 394 and name CB)	14.96	0.56	0.57
70	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 395 and name CA)	17.26	0.74	0.75
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 396 and name CA)	17.26	0.82	0.82
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 396 and name CB)	16.26	0.84	0.84
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 397 and name CA)	17.73	0.82	0.83
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 397 and name CB)	16.91	0.80	0.79
75	assign (segid 3A4 and resid 67 and name CA) (segid HEM and resid 1 and name CAD)	5.71	0.54	0.55
	assign (segid 3A4 and resid 67 and name CA) (segid HEM and resid 1 and name CBD)	5.75	0.46	0.46
	assign (segid 3A4 and resid 67 and name CA) (segid HEM and resid 1 and name CGD)	5.01	0.43	0.44
	assign (segid 3A4 and resid 67 and name CA) (segid HEM and resid 1 and name CMD)	6.30	0.76	0.77
	assign (segid 3A4 and resid 67 and name CA) (segid HEM and resid 1 and name O1D)	5.00	0.55	0.54
	assign (segid 3A4 and resid 67 and name CA) (segid HEM and resid 1 and name O2D)	4.91	0.45	0.45
80	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 67 and name C)	1.52	0.01	0.01
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 67 and name CB)	1.53	0.03	0.02
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 67 and name O)	2.40	0.01	0.01

	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 68 and name C)	4.55	0.05	0.06
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 68 and name CA)	3.81	0.01	0.02
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 68 and name N)	2.45	0.02	0.02
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 68 and name O)	5.15	0.32	0.33
5	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 69 and name C)	5.74	0.26	0.26
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 69 and name CA)	5.76	0.30	0.29
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 69 and name N)	4.60	0.32	0.32
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 69 and name O)	6.50	0.49	0.50
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 70 and name C)	6.35	0.59	0.58
10	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 70 and name CA)	5.74	0.69	0.69
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 70 and name N)	5.23	0.71	0.71
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 70 and name O)	6.10	0.63	0.63
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 71 and name CA)	8.37	0.45	0.45
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 71 and name CB)	9.72	0.39	0.40
15	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 72 and name CA)	9.45	0.22	0.22
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 73 and name CA)	10.76	0.35	0.34
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 73 and name CB)	12.00	0.36	0.35
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 74 and name C)	6.82	0.43	0.42
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 74 and name CA)	8.08	0.43	0.43
20	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 74 and name CB)	7.91	0.43	0.43
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 74 and name O)	6.48	0.53	0.54
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 75 and name C)	6.02	0.38	0.38
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 75 and name CA)	5.44	0.31	0.32
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 75 and name CB)	5.70	0.28	0.27
25	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 75 and name CG)	5.35	0.33	0.33
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 75 and name N)	6.42	0.33	0.34
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 75 and name O)	5.56	0.43	0.43
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 76 and name CA)	8.20	0.41	0.41
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 76 and name CB)	9.61	0.40	0.41
30	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 76 and name N)	7.30	0.38	0.38
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 77 and name CA)	8.96	0.42	0.43
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 77 and name CB)	9.58	0.40	0.41
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 78 and name C)	5.98	0.46	0.47
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 78 and name CA)	6.14	0.45	0.44
35	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 78 and name CB)	5.02	0.41	0.40
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 78 and name N)	6.85	0.43	0.44
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 78 and name O)	6.48	0.61	0.62
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 79 and name CA)	6.16	0.40	0.39
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 79 and name CB)	6.17	0.37	0.36
40	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 79 and name CG)	7.00	0.37	0.37
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 79 and name N)	5.77	0.39	0.39
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 80 and name CA)	9.85	0.41	0.41
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 81 and name CA)	10.33	0.50	0.49
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 81 and name CB)	9.96	0.48	0.48
45	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 82 and name CB)	9.41	0.89	0.89
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 82 and name CB)	8.25	1.08	1.08
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 83 and name CA)	10.97	0.34	0.33
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 83 and name CB)	10.98	0.27	0.27
50	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 84 and name CA)	14.19	0.68	0.69
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 84 and name CB)	14.67	0.87	0.87
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 85 and name CA)	14.49	0.86	0.86
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 85 and name CB)	14.00	0.91	0.91
	assign (segid 3A4 and resid 67 and name CA) (segid 3A4 and resid 86 and name CA)	13.61	0.71	0.72
55	assign (segid 3A4 and resid 67 and name CB) (segid 3A4 and resid 86 and name CB)	12.36	0.69	0.69
	assign (segid 3A4 and resid 67 and name CB) (segid 3A4 and resid 134 and name CA)	17.12	0.84	0.83
	assign (segid 3A4 and resid 67 and name CB) (segid 3A4 and resid 137 and name CA)	16.47	1.78	1.78
	assign (segid 3A4 and resid 67 and name CB) (segid 3A4 and resid 138 and name CA)	16.59	0.58	0.59
	assign (segid 3A4 and resid 67 and name CB) (segid 3A4 and resid 138 and name CB)	16.34	0.68	0.68
60	assign (segid 3A4 and resid 67 and name CB) (segid 3A4 and resid 191 and name CB)	17.96	1.16	1.17
	assign (segid 3A4 and resid 67 and name CB) (segid 3A4 and resid 194 and name CB)	17.34	1.19	1.19
	assign (segid 3A4 and resid 67 and name CB) (segid 3A4 and resid 195 and name CA)	17.31	0.85	0.86
	assign (segid 3A4 and resid 67 and name CB) (segid 3A4 and resid 195 and name CB)	17.28	0.77	0.76
	assign (segid 3A4 and resid 67 and name CB) (segid 3A4 and resid 198 and name CA)	17.29	0.87	0.87
	assign (segid 3A4 and resid 67 and name CB) (segid 3A4 and resid 198 and name CB)	15.88	0.86	0.87
65	assign (segid 3A4 and resid 67 and name CB) (segid 3A4 and resid 199 and name CA)	18.60	0.72	0.72
	assign (segid 3A4 and resid 67 and name CB) (segid 3A4 and resid 199 and name CB)	19.16	0.77	0.77
	assign (segid 3A4 and resid 67 and name CB) (segid 3A4 and resid 202 and name CA)	18.14	0.40	0.41
	assign (segid 3A4 and resid 67 and name CB) (segid 3A4 and resid 202 and name CB)	17.15	0.44	0.44
70	assign (segid 3A4 and resid 67 and name CB) (segid 3A4 and resid 219 and name CA)	17.82	1.07	1.06
	assign (segid 3A4 and resid 67 and name CB) (segid 3A4 and resid 219 and name CB)	18.23	1.08	1.09
	assign (segid 3A4 and resid 67 and name CB) (segid 3A4 and resid 220 and name CA)	14.13	1.00	1.00
	assign (segid 3A4 and resid 67 and name CB) (segid 3A4 and resid 221 and name CA)	13.15	1.11	1.11
	assign (segid 3A4 and resid 67 and name CB) (segid 3A4 and resid 221 and name CB)	14.78	0.62	0.63
75	assign (segid 3A4 and resid 67 and name CB) (segid 3A4 and resid 221 and name CB)	15.61	0.64	0.63
	assign (segid 3A4 and resid 67 and name CB) (segid 3A4 and resid 222 and name CA)	17.42	0.52	0.51
	assign (segid 3A4 and resid 67 and name CB) (segid 3A4 and resid 222 and name CB)	18.63	0.56	0.56
	assign (segid 3A4 and resid 67 and name CB) (segid 3A4 and resid 223 and name CA)	15.45	0.57	0.57
	assign (segid 3A4 and resid 67 and name CB) (segid 3A4 and resid 223 and name CB)	14.86	0.72	0.71
	assign (segid 3A4 and resid 67 and name CB) (segid 3A4 and resid 224 and name CA)	12.87	0.41	0.40
80	assign (segid 3A4 and resid 67 and name CB) (segid 3A4 and resid 224 and name CB)	11.96	0.38	0.39
	assign (segid 3A4 and resid 67 and name CB) (segid 3A4 and resid 225 and name CA)	15.86	0.53	0.53
	assign (segid 3A4 and resid 67 and name CB) (segid 3A4 and resid 225 and name CB)	16.92	0.51	0.51
	assign (segid 3A4 and resid 67 and name CB) (segid 3A4 and resid 226 and name CA)	17.70	0.59	0.59

5	assign	(segid 3A4 and resid 67 and name CB)	(segid 3A4 and resid 240 and name CA)	14.29	0.33	0.34
	assign	(segid 3A4 and resid 67 and name CB)	(segid 3A4 and resid 240 and name CB)	14.40	0.31	0.31
	assign	(segid 3A4 and resid 67 and name CB)	(segid 3A4 and resid 241 and name CA)	15.19	0.31	0.31
	assign	(segid 3A4 and resid 67 and name CB)	(segid 3A4 and resid 241 and name CB)	16.61	0.31	0.32
	assign	(segid 3A4 and resid 67 and name CB)	(segid 3A4 and resid 242 and name CA)	13.58	0.41	0.41
10	assign	(segid 3A4 and resid 67 and name CB)	(segid 3A4 and resid 242 and name CB)	14.06	0.43	0.42
	assign	(segid 3A4 and resid 67 and name CB)	(segid 3A4 and resid 243 and name CA)	10.10	0.33	0.34
	assign	(segid 3A4 and resid 67 and name CB)	(segid 3A4 and resid 243 and name CB)	9.87	0.30	0.31
	assign	(segid 3A4 and resid 67 and name CB)	(segid 3A4 and resid 244 and name CA)	10.89	0.60	0.59
	assign	(segid 3A4 and resid 67 and name CB)	(segid 3A4 and resid 244 and name CB)	12.22	0.57	0.57
15	assign	(segid 3A4 and resid 67 and name CB)	(segid 3A4 and resid 245 and name CA)	12.16	0.78	0.77
	assign	(segid 3A4 and resid 67 and name CB)	(segid 3A4 and resid 245 and name CB)	13.30	0.75	0.75
	assign	(segid 3A4 and resid 67 and name CB)	(segid 3A4 and resid 246 and name CA)	9.38	0.67	0.68
	assign	(segid 3A4 and resid 67 and name CB)	(segid 3A4 and resid 246 and name CB)	9.02	0.53	0.53
	assign	(segid 3A4 and resid 67 and name CB)	(segid 3A4 and resid 247 and name CA)	7.06	0.81	0.80
20	assign	(segid 3A4 and resid 67 and name CB)	(segid 3A4 and resid 247 and name CB)	6.93	0.70	0.71
	assign	(segid 3A4 and resid 67 and name CB)	(segid 3A4 and resid 248 and name CA)	10.33	0.95	0.95
	assign	(segid 3A4 and resid 67 and name CB)	(segid 3A4 and resid 248 and name CB)	11.64	0.92	0.92
	assign	(segid 3A4 and resid 67 and name CB)	(segid 3A4 and resid 249 and name CA)	11.01	1.05	1.05
	assign	(segid 3A4 and resid 67 and name CB)	(segid 3A4 and resid 250 and name CA)	8.16	1.12	1.11
25	assign	(segid 3A4 and resid 67 and name CB)	(segid 3A4 and resid 250 and name CB)	6.73	1.09	1.08
	assign	(segid 3A4 and resid 67 and name CB)	(segid 3A4 and resid 251 and name CA)	9.16	1.16	1.16
	assign	(segid 3A4 and resid 67 and name CB)	(segid 3A4 and resid 251 and name CB)	9.35	1.09	1.08
	assign	(segid 3A4 and resid 67 and name CB)	(segid 3A4 and resid 252 and name CA)	12.67	1.16	1.15
	assign	(segid 3A4 and resid 67 and name CB)	(segid 3A4 and resid 252 and name CB)	13.38	1.12	1.13
30	assign	(segid 3A4 and resid 67 and name CB)	(segid 3A4 and resid 253 and name CA)	12.72	1.18	1.17
	assign	(segid 3A4 and resid 67 and name CB)	(segid 3A4 and resid 254 and name CA)	10.95	1.09	1.09
	assign	(segid 3A4 and resid 67 and name CB)	(segid 3A4 and resid 255 and name CA)	13.03	1.38	1.37
	assign	(segid 3A4 and resid 67 and name CB)	(segid 3A4 and resid 256 and name CA)	16.18	1.26	1.25
	assign	(segid 3A4 and resid 67 and name CB)	(segid 3A4 and resid 257 and name CA)	17.40	1.18	1.18
35	assign	(segid 3A4 and resid 67 and name CB)	(segid 3A4 and resid 258 and name CA)	16.70	1.17	1.17
	assign	(segid 3A4 and resid 67 and name CB)	(segid 3A4 and resid 258 and name CB)	15.39	1.18	1.17
	assign	(segid 3A4 and resid 67 and name CB)	(segid 3A4 and resid 319 and name CA)	16.89	0.82	0.83
	assign	(segid 3A4 and resid 67 and name CB)	(segid 3A4 and resid 319 and name CB)	15.49	0.83	0.84
	assign	(segid 3A4 and resid 67 and name CB)	(segid 3A4 and resid 322 and name CA)	14.97	0.44	0.45
40	assign	(segid 3A4 and resid 67 and name CB)	(segid 3A4 and resid 323 and name CA)	14.96	0.63	0.64
	assign	(segid 3A4 and resid 67 and name CB)	(segid 3A4 and resid 323 and name CB)	15.26	0.74	0.74
	assign	(segid 3A4 and resid 67 and name CB)	(segid 3A4 and resid 324 and name CA)	17.00	0.67	0.66
	assign	(segid 3A4 and resid 67 and name CB)	(segid 3A4 and resid 324 and name CB)	16.72	0.64	0.65
	assign	(segid 3A4 and resid 67 and name CB)	(segid 3A4 and resid 344 and name CA)	19.24	0.39	0.40
45	assign	(segid 3A4 and resid 67 and name CB)	(segid 3A4 and resid 345 and name CA)	18.88	0.80	0.80
	assign	(segid 3A4 and resid 67 and name CB)	(segid 3A4 and resid 345 and name CB)	17.88	0.94	0.93
	assign	(segid 3A4 and resid 67 and name CB)	(segid 3A4 and resid 347 and name CB)	18.26	0.95	0.95
	assign	(segid 3A4 and resid 67 and name CB)	(segid 3A4 and resid 382 and name CA)	18.45	0.61	0.61
	assign	(segid 3A4 and resid 67 and name CB)	(segid 3A4 and resid 382 and name CB)	18.51	0.66	0.66
50	assign	(segid 3A4 and resid 67 and name CB)	(segid 3A4 and resid 383 and name CA)	17.65	0.70	0.70
	assign	(segid 3A4 and resid 67 and name CB)	(segid 3A4 and resid 384 and name CA)	14.28	0.64	0.63
	assign	(segid 3A4 and resid 67 and name CB)	(segid 3A4 and resid 384 and name CB)	14.30	0.62	0.62
	assign	(segid 3A4 and resid 67 and name CB)	(segid 3A4 and resid 385 and name CA)	13.65	0.68	0.68
	assign	(segid 3A4 and resid 67 and name CB)	(segid 3A4 and resid 386 and name CA)	14.20	0.61	0.61
55	assign	(segid 3A4 and resid 67 and name CB)	(segid 3A4 and resid 387 and name			

	assign (segid 3A4 and resid 67 and name CB) (segid 3A4 and resid 71 and name CA)	9.13	0.77	0.78
	assign (segid 3A4 and resid 67 and name CB) (segid 3A4 and resid 71 and name CB)	10.55	0.70	0.71
	assign (segid 3A4 and resid 67 and name CB) (segid 3A4 and resid 72 and name CA)	9.76	0.47	0.46
	assign (segid 3A4 and resid 67 and name CB) (segid 3A4 and resid 73 and name CA)	11.00	0.74	0.74
5	assign (segid 3A4 and resid 67 and name CB) (segid 3A4 and resid 73 and name CB)	12.24	0.65	0.65
	assign (segid 3A4 and resid 67 and name CB) (segid 3A4 and resid 74 and name CA)	8.49	0.59	0.59
	assign (segid 3A4 and resid 67 and name CB) (segid 3A4 and resid 74 and name CB)	8.54	0.52	0.52
	assign (segid 3A4 and resid 67 and name CB) (segid 3A4 and resid 74 and name O)	6.64	0.67	0.67
	assign (segid 3A4 and resid 67 and name CB) (segid 3A4 and resid 75 and name C)	5.85	0.83	0.83
10	assign (segid 3A4 and resid 67 and name CB) (segid 3A4 and resid 75 and name CA)	5.62	0.72	0.71
	assign (segid 3A4 and resid 67 and name CB) (segid 3A4 and resid 75 and name CB)	5.92	0.72	0.73
	assign (segid 3A4 and resid 67 and name CB) (segid 3A4 and resid 75 and name CG)	5.35	0.78	0.78
	assign (segid 3A4 and resid 67 and name CB) (segid 3A4 and resid 75 and name N)	6.76	0.65	0.65
	assign (segid 3A4 and resid 67 and name CB) (segid 3A4 and resid 75 and name O)	5.17	0.90	0.90
15	assign (segid 3A4 and resid 67 and name CB) (segid 3A4 and resid 76 and name CA)	7.79	0.88	0.87
	assign (segid 3A4 and resid 67 and name CB) (segid 3A4 and resid 76 and name CB)	9.25	0.88	0.88
	assign (segid 3A4 and resid 67 and name CB) (segid 3A4 and resid 77 and name CA)	8.58	0.76	0.75
	assign (segid 3A4 and resid 67 and name CB) (segid 3A4 and resid 77 and name CB)	9.38	0.71	0.71
	assign (segid 3A4 and resid 67 and name CB) (segid 3A4 and resid 78 and name C)	5.25	0.60	0.61
20	assign (segid 3A4 and resid 67 and name CB) (segid 3A4 and resid 78 and name CA)	5.70	0.65	0.64
	assign (segid 3A4 and resid 67 and name CB) (segid 3A4 and resid 78 and name CB)	4.85	0.59	0.59
	assign (segid 3A4 and resid 67 and name CB) (segid 3A4 and resid 78 and name N)	6.49	0.73	0.73
	assign (segid 3A4 and resid 67 and name CB) (segid 3A4 and resid 78 and name O)	5.65	0.63	0.62
25	assign (segid 3A4 and resid 67 and name CB) (segid 3A4 and resid 79 and name C)	6.55	0.56	0.56
	assign (segid 3A4 and resid 67 and name CB) (segid 3A4 and resid 79 and name CA)	5.12	0.58	0.59
	assign (segid 3A4 and resid 67 and name CB) (segid 3A4 and resid 79 and name CB)	5.17	0.68	0.69
	assign (segid 3A4 and resid 67 and name CB) (segid 3A4 and resid 79 and name CG)	5.91	0.62	0.61
	assign (segid 3A4 and resid 67 and name CB) (segid 3A4 and resid 79 and name N)	4.95	0.67	0.67
30	assign (segid 3A4 and resid 67 and name CB) (segid 3A4 and resid 80 and name CA)	8.85	0.60	0.60
	assign (segid 3A4 and resid 67 and name CB) (segid 3A4 and resid 81 and name CA)	9.43	0.54	0.53
	assign (segid 3A4 and resid 67 and name CB) (segid 3A4 and resid 81 and name CB)	9.21	0.54	0.53
	assign (segid 3A4 and resid 67 and name CB) (segid 3A4 and resid 82 and name CA)	8.31	0.80	0.79
	assign (segid 3A4 and resid 67 and name CB) (segid 3A4 and resid 82 and name CB)	7.16	1.01	1.00
35	assign (segid 3A4 and resid 67 and name CB) (segid 3A4 and resid 83 and name CA)	9.68	0.26	0.25
	assign (segid 3A4 and resid 67 and name CB) (segid 3A4 and resid 83 and name CB)	9.71	0.27	0.26
	assign (segid 3A4 and resid 67 and name CB) (segid 3A4 and resid 84 and name CA)	12.95	0.56	0.56
	assign (segid 3A4 and resid 67 and name CB) (segid 3A4 and resid 84 and name CB)	13.50	0.74	0.73
	assign (segid 3A4 and resid 67 and name CB) (segid 3A4 and resid 85 and name CA)	13.32	0.75	0.75
40	assign (segid 3A4 and resid 67 and name CB) (segid 3A4 and resid 85 and name CB)	12.91	0.80	0.80
	assign (segid 3A4 and resid 67 and name CB) (segid 3A4 and resid 86 and name CA)	12.35	0.74	0.74
	assign (segid 3A4 and resid 67 and name CB) (segid 3A4 and resid 86 and name CB)	11.12	0.78	0.77
	assign (segid 3A4 and resid 67 and name N) (segid 3A4 and resid 246 and name C)	6.47	0.69	0.69
	assign (segid 3A4 and resid 67 and name N) (segid 3A4 and resid 246 and name CB)	6.90	0.53	0.53
45	assign (segid 3A4 and resid 67 and name N) (segid 3A4 and resid 246 and name O)	6.26	0.82	0.81
	assign (segid 3A4 and resid 67 and name N) (segid 3A4 and resid 247 and name CA)	5.79	0.66	0.65
	assign (segid 3A4 and resid 67 and name N) (segid 3A4 and resid 247 and name CB)	5.94	0.61	0.61
	assign (segid 3A4 and resid 67 and name N) (segid 3A4 and resid 247 and name N)	6.25	0.61	0.60
	assign (segid 3A4 and resid 67 and name N) (segid 3A4 and resid 250 and name CB)	5.61	0.74	0.75
50	assign (segid 3A4 and resid 67 and name N) (segid HEM and resid 1 and name CAD)	6.29	0.58	0.57
	assign (segid 3A4 and resid 67 and name N) (segid HEM and resid 1 and name CBD)	6.55	0.50	0.51
	assign (segid 3A4 and resid 67 and name N) (segid HEM and resid 1 and name CGD)	6.04	0.56	0.55
	assign (segid 3A4 and resid 67 and name N) (segid HEM and resid 1 and name CMD)	6.34	0.58	0.58
	assign (segid 3A4 and resid 67 and name N) (segid HEM and resid 1 and name O1D)	6.10	0.60	0.61
	assign (segid 3A4 and resid 67 and name N) (segid HEM and resid 1 and name O2D)	5.96	0.61	0.61
55	assign (segid 3A4 and resid 67 and name N) (segid 3A4 and resid 67 and name C)	2.54	0.03	0.02
	assign (segid 3A4 and resid 67 and name N) (segid 3A4 and resid 67 and name CA)	1.46	0.01	0.00
	assign (segid 3A4 and resid 67 and name N) (segid 3A4 and resid 67 and name CB)	2.43	0.05	0.04
	assign (segid 3A4 and resid 67 and name N) (segid 3A4 and resid 67 and name O)	3.59	0.05	0.06
60	assign (segid 3A4 and resid 67 and name N) (segid 3A4 and resid 68 and name C)	5.00	0.11	0.11
	assign (segid 3A4 and resid 67 and name N) (segid 3A4 and resid 68 and name CA)	4.33	0.07	0.07
	assign (segid 3A4 and resid 67 and name N) (segid 3A4 and resid 68 and name N)	2.90	0.08	0.08
	assign (segid 3A4 and resid 67 and name N) (segid 3A4 and resid 68 and name O)	5.93	0.53	0.53
	assign (segid 3A4 and resid 67 and name N) (segid 3A4 and resid 69 and name C)	6.07	0.34	0.34
	assign (segid 3A4 and resid 67 and name N) (segid 3A4 and resid 69 and name CA)	5.99	0.36	0.35
65	assign (segid 3A4 and resid 67 and name N) (segid 3A4 and resid 69 and name N)	4.89	0.39	0.38
	assign (segid 3A4 and resid 67 and name N) (segid 3A4 and resid 70 and name C)	7.16	0.37	0.37
	assign (segid 3A4 and resid 67 and name N) (segid 3A4 and resid 70 and name CA)	6.34	0.53	0.52
	assign (segid 3A4 and resid 67 and name N) (segid 3A4 and resid 70 and name N)	5.77	0.59	0.58
	assign (segid 3A4 and resid 67 and name N) (segid 3A4 and resid 75 and name C)	6.95	0.33	0.34
70	assign (segid 3A4 and resid 67 and name N) (segid 3A4 and resid 75 and name CA)	6.37	0.33	0.33
	assign (segid 3A4 and resid 67 and name N) (segid 3A4 and resid 75 and name CB)	6.78	0.19	0.20
	assign (segid 3A4 and resid 67 and name N) (segid 3A4 and resid 75 and name CG)	6.58	0.22	0.23
	assign (segid 3A4 and resid 67 and name N) (segid 3A4 and resid 75 and name O)	6.43	0.38	0.39
	assign (segid 3A4 and resid 67 and name N) (segid 3A4 and resid 78 and name C)	6.27	0.53	0.54
75	assign (segid 3A4 and resid 67 and name N) (segid 3A4 and resid 78 and name CA)	6.30	0.48	0.49
	assign (segid 3A4 and resid 67 and name N) (segid 3A4 and resid 78 and name CB)	5.07	0.46	0.45
	assign (segid 3A4 and resid 67 and name N) (segid 3A4 and resid 78 and name O)	6.63	0.69	0.69
	assign (segid 3A4 and resid 67 and name N) (segid 3A4 and resid 79 and name CA)	6.80	0.50	0.49
	assign (segid 3A4 and resid 67 and name N) (segid 3A4 and resid 79 and name N)	6.33	0.47	0.46
80	assign (segid 3A4 and resid 67 and name O) (segid 3A4 and resid 389 and name CA)	6.86	0.35	0.36
	assign (segid 3A4 and resid 67 and name O) (segid 3A4 and resid 389 and name CB)	6.47	0.51	0.51
	assign (segid 3A4 and resid 67 and name O) (segid 3A4 and resid 389 and name O)	7.56	0.23	0.24
	assign (segid 3A4 and resid 67 and name O) (segid HEM and resid 1 and name C3D)	6.89	0.68	0.69

	assign	(segid 3A4 and resid 67 and name O)	(segid HEM and resid 1 and name CAD)	5.47	0.62	0.63
	assign	(segid 3A4 and resid 67 and name O)	(segid HEM and resid 1 and name CBD)	5.40	0.53	0.53
	assign	(segid 3A4 and resid 67 and name O)	(segid HEM and resid 1 and name CGD)	1.27	0.37	0.37
	assign	(segid 3A4 and resid 67 and name O)	(segid HEM and resid 1 and name OLD)	4.27	0.53	0.53
5	assign	(segid 3A4 and resid 67 and name O)	(segid HEM and resid 1 and name O2D)	3.82	0.35	0.34
	assign	(segid 3A4 and resid 67 and name O)	(segid 3A4 and resid 67 and name CB)	3.18	0.11	0.12
	assign	(segid 3A4 and resid 67 and name O)	(segid 3A4 and resid 68 and name C)	3.13	0.09	0.10
	assign	(segid 3A4 and resid 67 and name O)	(segid 3A4 and resid 68 and name CA)	2.74	0.02	0.03
	assign	(segid 3A4 and resid 67 and name O)	(segid 3A4 and resid 68 and name N)	2.24	0.02	0.02
10	assign	(segid 3A4 and resid 67 and name O)	(segid 3A4 and resid 68 and name O)	3.85	0.15	0.15
	assign	(segid 3A4 and resid 67 and name O)	(segid 3A4 and resid 69 and name C)	4.43	0.24	0.24
	assign	(segid 3A4 and resid 67 and name O)	(segid 3A4 and resid 69 and name CA)	4.49	0.20	0.20
	assign	(segid 3A4 and resid 67 and name O)	(segid 3A4 and resid 69 and name N)	3.43	0.18	0.17
	assign	(segid 3A4 and resid 67 and name O)	(segid 3A4 and resid 69 and name O)	5.34	0.39	0.40
15	assign	(segid 3A4 and resid 67 and name O)	(segid 3A4 and resid 70 and name C)	4.67	0.67	0.68
	assign	(segid 3A4 and resid 67 and name O)	(segid 3A4 and resid 70 and name CA)	4.40	0.69	0.70
	assign	(segid 3A4 and resid 67 and name O)	(segid 3A4 and resid 70 and name N)	3.76	0.68	0.69
	assign	(segid 3A4 and resid 67 and name O)	(segid 3A4 and resid 70 and name O)	4.14	0.73	0.74
	assign	(segid 3A4 and resid 67 and name O)	(segid 3A4 and resid 71 and name C)	6.93	0.34	0.35
20	assign	(segid 3A4 and resid 67 and name O)	(segid 3A4 and resid 71 and name N)	5.89	0.60	0.60
	assign	(segid 3A4 and resid 67 and name O)	(segid 3A4 and resid 71 and name O)	6.81	0.27	0.27
	assign	(segid 3A4 and resid 67 and name O)	(segid 3A4 and resid 74 and name C)	7.00	0.34	0.33
	assign	(segid 3A4 and resid 67 and name O)	(segid 3A4 and resid 74 and name O)	7.03	0.37	0.37
	assign	(segid 3A4 and resid 67 and name O)	(segid 3A4 and resid 75 and name C)	6.02	0.39	0.38
25	assign	(segid 3A4 and resid 67 and name O)	(segid 3A4 and resid 75 and name CA)	5.17	0.35	0.35
	assign	(segid 3A4 and resid 67 and name O)	(segid 3A4 and resid 75 and name CB)	4.78	0.33	0.34
	assign	(segid 3A4 and resid 67 and name O)	(segid 3A4 and resid 75 and name CG)	4.27	0.33	0.33
	assign	(segid 3A4 and resid 67 and name O)	(segid 3A4 and resid 75 and name N)	6.20	0.34	0.35
	assign	(segid 3A4 and resid 67 and name O)	(segid 3A4 and resid 75 and name O)	5.95	0.39	0.40
30	assign	(segid 3A4 and resid 67 and name O)	(segid 3A4 and resid 76 and name N)	7.14	0.40	0.40
	assign	(segid 3A4 and resid 67 and name O)	(segid 3A4 and resid 78 and name CB)	6.70	0.37	0.36
	assign	(segid 3A4 and resid 67 and name O)	(segid 3A4 and resid 79 and name CA)	7.20	0.47	0.46
	assign	(segid 3A4 and resid 67 and name O)	(segid 3A4 and resid 79 and name CB)	6.70	0.45	0.45
	assign	(segid 3A4 and resid 67 and name O)	(segid 3A4 and resid 79 and name N)	6.96	0.41	0.41
35	assign	(segid 3A4 and resid 68 and name C)	(segid HEM and resid 1 and name CAD)	5.95	0.54	0.53
	assign	(segid 3A4 and resid 68 and name C)	(segid HEM and resid 1 and name CBD)	6.53	0.42	0.42
	assign	(segid 3A4 and resid 68 and name C)	(segid HEM and resid 1 and name CGD)	5.78	0.31	0.31
	assign	(segid 3A4 and resid 68 and name C)	(segid HEM and resid 1 and name OLD)	6.16	0.72	0.72
	assign	(segid 3A4 and resid 68 and name C)	(segid HEM and resid 1 and name O2D)	5.08	0.55	0.56
40	assign	(segid 3A4 and resid 68 and name C)	(segid 3A4 and resid 68 and name O)	1.24	0.01	0.01
	assign	(segid 3A4 and resid 68 and name C)	(segid 3A4 and resid 69 and name C)	3.34	0.13	0.12
	assign	(segid 3A4 and resid 68 and name C)	(segid 3A4 and resid 69 and name CA)	2.42	0.03	0.03
	assign	(segid 3A4 and resid 68 and name C)	(segid 3A4 and resid 69 and name N)	1.33	0.00	0.01
	assign	(segid 3A4 and resid 68 and name C)	(segid 3A4 and resid 69 and name O)	4.28	0.46	0.46
45	assign	(segid 3A4 and resid 68 and name C)	(segid 3A4 and resid 70 and name C)	5.45	0.40	0.40
	assign	(segid 3A4 and resid 68 and name C)	(segid 3A4 and resid 70 and name CA)	4.87	0.26	0.26
	assign	(segid 3A4 and resid 68 and name C)	(segid 3A4 and resid 70 and name N)	3.55	0.31	0.32
	assign	(segid 3A4 and resid 68 and name C)	(segid 3A4 and resid 70 and name O)	5.09	0.51	0.50
	assign	(segid 3A4 and resid 68 and name C)	(segid 3A4 and resid 71 and name N)	6.70	0.37	0.38
50	assign	(segid 3A4 and resid 68 and name C)	(segid 3A4 and resid 75 and name CG)	6.98	0.39	0.39
	assign	(segid 3A4 and resid 68 and name CA)	(segid 3A4 and resid 134 and name CA)	18.25	0.46	0.46
	assign	(segid 3A4 and resid 68 and name CA)	(segid 3A4 and resid 157 and name CA)	17.30	0.88	0.89
	assign	(segid 3A4 and resid 68 and name CA)	(segid 3A4 and resid 157 and name CB)	17.54	0.82	0.81
	assign	(segid 3A4 and resid 68 and name CA)	(segid 3A4 and resid 160 and name CA)	16.40	1.74	1.75
55	assign	(segid 3A4 and resid 68 and name CA)	(segid 3A4 and resid 160 and name CB)	15.77	1.69	1.68
	assign	(segid 3A4 and resid 68 and name CA)	(segid 3A4 and resid 161 and name CA)	16.98	1.42	1.42
	assign	(segid 3A4 and resid 68 and name CA)	(segid 3A4 and resid 191 and name CA)	16.82	1.13	1.13
	assign	(segid 3A4 and resid 68 and name CA)	(segid 3A4 and resid 191 and name CB)	16.15	1.14	1.15
	assign	(segid 3A4 and resid 68 and name CA)	(segid 3A4 and resid 194 and name CA)	17.85	1.07	1.07
60	assign	(segid 3A4 and resid 68 and name CA)	(segid 3A4 and resid 194 and name CB)	16.61	1.13	1.14
	assign	(segid 3A4 and resid 68 and name CA)	(segid 3A4 and resid 195 and name CA)	17.23	0.81	0.81
	assign	(segid 3A4 and resid 68 and name CA)	(segid 3A4 and resid 195 and name CB)	17.03	0.78	0.77
	assign	(segid 3A4 and resid 68 and name CA)	(segid 3A4 and resid 198 and name CB)	16.81	0.78	0.78
	assign	(segid 3A4 and resid 68 and name CA)	(segid 3A4 and resid 220 and name CA)	17.32	0.67	0.66
65	assign	(segid 3A4 and resid 68 and name CA)	(segid 3A4 and resid 220 and name CB)	16.16	0.74	0.74
	assign	(segid 3A4 and resid 68 and name CA)	(segid 3A4 and resid 221 and name CA)	17.80	0.51	0.51
	assign	(segid 3A4 and resid 68 and name CA)	(segid 3A4 and resid 221 and name CB)	18.36	0.60	0.60
	assign	(segid 3A4 and resid 68 and name CA)	(segid 3A4 and resid 223 and name CB)	18.71	0.54	0.55
	assign	(segid 3A4 and resid 68 and name CA)	(segid 3A4 and resid 224 and name CA)	16.63	0.53	0.53
70	assign	(segid 3A4 and resid 68 and name CA)	(segid 3A4 and resid 224 and name CB)	15.54	0.53	0.52
	assign	(segid 3A4 and resid 68 and name CA)	(segid 3A4 and resid 240 and name CA)	16.97	0.30	0.31
	assign	(segid 3A4 and resid 68 and name CA)	(segid 3A4 and resid 240 and name CB)	16.80	0.36	0.35
	assign	(segid 3A4 and resid 68 and name CA)	(segid 3A4 and resid 241 and name CA)	17.48	0.30	0.29
	assign	(segid 3A4 and resid 68 and name CA)	(segid 3A4 and resid 241 and name CB)	18.77	0.33	0.33
75	assign	(segid 3A4 and resid 68 and name CA)	(segid 3A4 and resid 242 and name CA)	15.04	0.47	0.48
	assign	(segid 3A4 and resid 68 and name CA)	(segid 3A4 and resid 242 and name CB)	15.29	0.56	0.55
	assign	(segid 3A4 and resid 68 and name CA)	(segid 3A4 and resid 243 and name CA)	12.15	0.37	0.37
	assign	(segid 3A4 and resid 68 and name CA)	(segid 3A4 and resid 243 and name CB)	12.27	0.35	0.35
	assign	(segid 3A4 and resid 68 and name CA)	(segid 3A4 and resid 244 and name CA)	13.48	0.47	0.46
	assign	(segid 3A4 and resid 68 and name CA)	(segid 3A4 and resid 244 and name CB)	14.95	0.46	0.47
80	assign	(segid 3A4 and resid 68 and name CA)	(segid 3A4 and resid 245 and name CA)	13.65	0.57	0.57
	assign	(segid 3A4 and resid 68 and name CA)	(segid 3A4 and resid 245 and name CB)	14.54	0.59	0.59
	assign	(segid 3A4 and resid 68 and name CA)	(segid 3A4 and resid 246 and name CA)	10.14	0.54	0.53

	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 246 and name CB)	9.63	0.45	0.45
	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 247 and name CA)	9.03	0.59	0.58
	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 247 and name CB)	9.60	0.57	0.56
	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 248 and name CA)	11.95	0.69	0.70
5	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 248 and name CB)	13.35	0.68	0.67
	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 249 and name CA)	11.15	0.77	0.77
	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 250 and name CA)	7.85	0.82	0.81
	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 250 and name CB)	6.58	0.81	0.81
	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 251 and name CA)	9.98	0.81	0.81
10	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 251 and name CB)	10.78	0.73	0.74
	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 252 and name CA)	12.72	0.88	0.89
	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 252 and name CB)	13.45	0.86	0.86
	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 253 and name CA)	11.45	0.98	0.98
	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 254 and name CA)	9.61	1.05	1.05
15	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 255 and name CA)	12.57	1.15	1.16
	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 256 and name CA)	15.32	0.92	0.92
	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 257 and name CA)	15.62	0.80	0.81
	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 258 and name CA)	14.94	0.76	0.75
	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 258 and name CB)	13.68	0.74	0.74
20	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 259 and name CA)	17.38	0.81	0.81
	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 259 and name CB)	17.32	0.88	0.88
	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 317 and name CA)	18.66	0.69	0.69
	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 318 and name CA)	16.94	0.61	0.60
	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 318 and name CB)	16.90	0.77	0.78
25	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 319 and name CA)	13.78	0.63	0.62
	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 319 and name CB)	12.52	0.63	0.62
	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 322 and name CA)	10.87	0.61	0.61
	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 323 and name CA)	11.34	0.91	0.92
	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 323 and name CB)	11.88	1.01	1.01
30	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 324 and name CA)	13.61	0.95	0.96
	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 324 and name CB)	13.34	0.96	0.96
	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 325 and name CA)	16.47	1.03	1.04
	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 326 and name CA)	16.97	0.99	0.98
	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 326 and name CB)	16.39	1.15	1.15
35	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 340 and name CA)	18.49	0.81	0.82
	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 342 and name CA)	16.19	0.64	0.65
	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 343 and name CA)	15.99	0.70	0.70
	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 343 and name CB)	16.03	0.78	0.79
	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 344 and name CA)	15.24	0.46	0.47
40	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 344 and name CB)	15.96	0.32	0.31
	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 345 and name CA)	15.33	0.88	0.88
	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 345 and name CB)	14.52	1.05	1.04
	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 346 and name CA)	17.18	0.92	0.92
	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 347 and name CA)	16.55	0.98	0.98
45	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 347 and name CB)	15.38	0.93	0.94
	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 382 and name CA)	16.72	0.61	0.62
	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 382 and name CB)	16.56	0.68	0.68
	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 383 and name CA)	15.81	0.52	0.53
	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 384 and name CA)	13.04	0.38	0.38
50	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 384 and name CB)	13.53	0.32	0.32
	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 385 and name CA)	11.90	0.64	0.64
	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 386 and name CA)	13.09	0.64	0.63
	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 387 and name CA)	12.52	0.58	0.58
	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 388 and name CA)	10.44	0.78	0.77
55	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 388 and name CB)	10.50	1.03	1.04
	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 389 and name CA)	7.37	0.62	0.62
	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 389 and name CB)	6.69	0.87	0.87
	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 389 and name O)	7.33	0.36	0.35
	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 390 and name CA)	9.86	0.27	0.27
60	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 390 and name CB)	11.24	0.27	0.26
	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 391 and name CA)	9.53	0.32	0.33
	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 391 and name CB)	10.48	0.36	0.36
	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 392 and name CA)	10.11	0.50	0.49
	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 392 and name CB)	9.27	0.56	0.56
65	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 393 and name CA)	12.28	0.62	0.63
	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 394 and name CA)	14.42	0.50	0.50
	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 394 and name CB)	14.43	0.40	0.39
	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 395 and name CA)	17.40	0.56	0.55
	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 396 and name CA)	17.44	0.69	0.68
70	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 396 and name CB)	16.58	0.73	0.72
	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 397 and name CA)	17.09	0.71	0.71
	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 397 and name CB)	16.03	0.70	0.70
	assign (segid 3A4 and resid 68 and name CA) (segid HEM and resid 1 and name C2D)	6.44	0.72	0.72
75	assign (segid 3A4 and resid 68 and name CA) (segid HEM and resid 1 and name C3D)	5.75	0.59	0.59
	assign (segid 3A4 and resid 68 and name CA) (segid HEM and resid 1 and name C4D)	6.69	0.52	0.51
	assign (segid 3A4 and resid 68 and name CA) (segid HEM and resid 1 and name CBD)	4.56	0.49	0.49
	assign (segid 3A4 and resid 68 and name CA) (segid HEM and resid 1 and name CGD)	5.20	0.37	0.37
	assign (segid 3A4 and resid 68 and name CA) (segid HEM and resid 1 and name CHA)	4.61	0.26	0.27
80	assign (segid 3A4 and resid 68 and name CA) (segid HEM and resid 1 and name CMD)	6.73	0.41	0.41
	assign (segid 3A4 and resid 68 and name CA) (segid HEM and resid 1 and name O1D)	6.34	0.83	0.83
	assign (segid 3A4 and resid 68 and name CA) (segid HEM and resid 1 and name O2D)	5.06	0.77	0.76
	assign (segid 3A4 and resid 68 and name CA) (segid HEM and resid 68 and name C)	4.05	0.50	0.49
	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 68 and name C)	1.51	0.01	0.02

	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 68 and name O)	2.39	0.02	0.02
	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 69 and name C)	4.62	0.08	0.08
	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 69 and name CA)	3.79	0.01	0.01
	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 69 and name N)	2.43	0.03	0.02
5	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 69 and name O)	5.59	0.45	0.45
	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 70 and name C)	6.30	0.46	0.46
	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 70 and name CA)	5.81	0.35	0.35
	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 70 and name N)	4.61	0.38	0.38
	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 70 and name O)	5.79	0.58	0.57
10	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 71 and name CA)	8.49	0.49	0.50
	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 71 and name CB)	9.69	0.56	0.56
	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 72 and name CA)	10.55	0.34	0.35
	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 73 and name CA)	12.80	0.31	0.32
	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 73 and name CB)	14.10	0.36	0.36
15	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 74 and name CA)	10.67	0.25	0.25
	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 74 and name CB)	10.31	0.23	0.23
	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 75 and name CA)	7.85	0.30	0.30
	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 75 and name CB)	7.38	0.32	0.31
	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 75 and name CG)	6.77	0.41	0.41
20	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 76 and name CA)	10.80	0.48	0.47
	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 76 and name CB)	12.02	0.49	0.48
	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 77 and name CA)	12.36	0.44	0.43
	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 77 and name CB)	13.00	0.38	0.38
	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 78 and name CA)	9.85	0.46	0.45
25	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 78 and name CB)	8.75	0.38	0.39
	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 79 and name CA)	9.16	0.55	0.56
	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 79 and name CB)	8.75	0.58	0.58
	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 80 and name CA)	12.95	0.57	0.56
	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 81 and name CA)	13.78	0.60	0.60
30	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 81 and name CB)	13.55	0.59	0.59
	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 82 and name CA)	12.30	0.90	0.91
	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 82 and name CB)	11.03	1.07	1.06
	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 83 and name CA)	13.33	0.47	0.47
	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 83 and name CB)	13.33	0.51	0.50
35	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 84 and name CA)	16.80	0.58	0.58
	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 84 and name CB)	17.48	0.75	0.75
	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 85 and name CA)	16.90	0.69	0.69
	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 85 and name CB)	16.50	0.72	0.72
	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 86 and name CA)	15.32	0.50	0.49
40	assign (segid 3A4 and resid 68 and name CA) (segid 3A4 and resid 86 and name CB)	13.92	0.45	0.45
	assign (segid 3A4 and resid 68 and name N) (segid 3A4 and resid 250 and name CB)	5.92	0.82	0.83
	assign (segid 3A4 and resid 68 and name N) (segid HEM and resid 1 and name C2D)	6.33	0.61	0.61
	assign (segid 3A4 and resid 68 and name N) (segid HEM and resid 1 and name C3D)	5.87	0.49	0.49
	assign (segid 3A4 and resid 68 and name N) (segid HEM and resid 1 and name C4D)	7.01	0.45	0.46
45	assign (segid 3A4 and resid 68 and name N) (segid HEM and resid 1 and name CAD)	4.69	0.38	0.38
	assign (segid 3A4 and resid 68 and name N) (segid HEM and resid 1 and name CBD)	5.20	0.28	0.29
	assign (segid 3A4 and resid 68 and name N) (segid HEM and resid 1 and name CGD)	4.61	0.22	0.22
	assign (segid 3A4 and resid 68 and name N) (segid HEM and resid 1 and name CMD)	5.90	0.74	0.74
	assign (segid 3A4 and resid 68 and name N) (segid HEM and resid 1 and name O1D)	4.93	0.69	0.69
50	assign (segid 3A4 and resid 68 and name N) (segid HEM and resid 1 and name O2D)	4.24	0.37	0.36
	assign (segid 3A4 and resid 68 and name N) (segid 3A4 and resid 68 and name C)	2.48	0.03	0.02
	assign (segid 3A4 and resid 68 and name N) (segid 3A4 and resid 68 and name O)	1.46	0.01	0.01
	assign (segid 3A4 and resid 68 and name N) (segid 3A4 and resid 68 and name CA)	3.46	0.25	0.24
	assign (segid 3A4 and resid 68 and name N) (segid 3A4 and resid 69 and name C)	4.86	0.08	0.07
55	assign (segid 3A4 and resid 68 and name N) (segid 3A4 and resid 69 and name CA)	4.29	0.18	0.18
	assign (segid 3A4 and resid 68 and name N) (segid 3A4 and resid 69 and name N)	2.89	0.23	0.23
	assign (segid 3A4 and resid 68 and name N) (segid 3A4 and resid 69 and name O)	5.77	0.45	0.44
	assign (segid 3A4 and resid 68 and name N) (segid 3A4 and resid 70 and name C)	6.35	0.49	0.49
	assign (segid 3A4 and resid 68 and name N) (segid 3A4 and resid 70 and name CA)	5.73	0.48	0.47
60	assign (segid 3A4 and resid 68 and name N) (segid 3A4 and resid 70 and name N)	4.69	0.54	0.54
	assign (segid 3A4 and resid 68 and name N) (segid 3A4 and resid 70 and name O)	5.95	0.60	0.60
	assign (segid 3A4 and resid 68 and name N) (segid 3A4 and resid 75 and name CA)	7.09	0.27	0.28
	assign (segid 3A4 and resid 68 and name N) (segid 3A4 and resid 75 and name CB)	6.89	0.26	0.25
	assign (segid 3A4 and resid 68 and name N) (segid 3A4 and resid 75 and name CG)	6.36	0.36	0.36
65	assign (segid 3A4 and resid 68 and name O) (segid HEM and resid 1 and name CAD)	6.42	0.62	0.62
	assign (segid 3A4 and resid 68 and name O) (segid HEM and resid 1 and name CBD)	7.00	0.51	0.50
	assign (segid 3A4 and resid 68 and name O) (segid HEM and resid 1 and name CGD)	6.23	0.45	0.45
	assign (segid 3A4 and resid 68 and name O) (segid HEM and resid 1 and name O1D)	6.63	0.77	0.76
	assign (segid 3A4 and resid 68 and name O) (segid HEM and resid 1 and name O2D)	5.47	0.71	0.71
70	assign (segid 3A4 and resid 68 and name O) (segid 3A4 and resid 69 and name C)	3.56	0.22	0.22
	assign (segid 3A4 and resid 68 and name O) (segid 3A4 and resid 69 and name CA)	2.76	0.03	0.02
	assign (segid 3A4 and resid 68 and name O) (segid 3A4 and resid 69 and name N)	2.26	0.01	0.02
	assign (segid 3A4 and resid 68 and name O) (segid 3A4 and resid 69 and name O)	4.33	0.63	0.63
	assign (segid 3A4 and resid 68 and name O) (segid 3A4 and resid 70 and name C)	5.49	0.51	0.51
75	assign (segid 3A4 and resid 68 and name O) (segid 3A4 and resid 70 and name CA)	5.10	0.28	0.28
	assign (segid 3A4 and resid 68 and name O) (segid 3A4 and resid 70 and name N)	3.87	0.30	0.29
	assign (segid 3A4 and resid 68 and name O) (segid 3A4 and resid 70 and name O)	5.07	0.68	0.69
	assign (segid 3A4 and resid 68 and name O) (segid 3A4 and resid 71 and name N)	6.65	0.48	0.49
	assign (segid 3A4 and resid 68 and name O) (segid 3A4 and resid 69 and name O)	1.24	0.01	0.01
80	assign (segid 3A4 and resid 69 and name C) (segid 3A4 and resid 70 and name C)	3.54	0.07	0.07
	assign (segid 3A4 and resid 69 and name C) (segid 3A4 and resid 70 and name CA)	2.45	0.02	0.02
	assign (segid 3A4 and resid 69 and name C) (segid 3A4 and resid 70 and name N)	1.33	0.01	0.01
	assign (segid 3A4 and resid 69 and name C) (segid 3A4 and resid 70 and name O)	3.94	0.09	0.08

	assign	(segid 3A4 and resid 69 and name C)	(segid 3A4 and resid 71 and name C)	6.73	0.08	0.07
	assign	(segid 3A4 and resid 69 and name C)	(segid 3A4 and resid 71 and name CA)	5.82	0.14	0.13
	assign	(segid 3A4 and resid 69 and name C)	(segid 3A4 and resid 71 and name CB)	6.61	0.25	0.25
	assign	(segid 3A4 and resid 69 and name C)	(segid 3A4 and resid 71 and name CG)	6.49	0.53	0.52
5	assign	(segid 3A4 and resid 69 and name C)	(segid 3A4 and resid 71 and name N)	4.52	0.13	0.14
	assign	(segid 3A4 and resid 69 and name C)	(segid 3A4 and resid 71 and name O)	6.68	0.06	0.06
	assign	(segid 3A4 and resid 69 and name C)	(segid 3A4 and resid 75 and name CB)	6.78	0.24	0.23
	assign	(segid 3A4 and resid 69 and name C)	(segid 3A4 and resid 75 and name CG)	7.05	0.23	0.23
	assign	(segid 3A4 and resid 69 and name CA)	(segid 3A4 and resid 160 and name CB)	16.13	1.79	1.79
10	assign	(segid 3A4 and resid 69 and name CA)	(segid 3A4 and resid 161 and name CB)	17.66	1.36	1.35
	assign	(segid 3A4 and resid 69 and name CA)	(segid 3A4 and resid 191 and name CA)	16.36	1.35	1.36
	assign	(segid 3A4 and resid 69 and name CA)	(segid 3A4 and resid 191 and name CB)	15.43	1.38	1.38
	assign	(segid 3A4 and resid 69 and name CA)	(segid 3A4 and resid 194 and name CB)	17.09	1.36	1.36
	assign	(segid 3A4 and resid 69 and name CA)	(segid 3A4 and resid 195 and name CA)	17.23	0.94	0.93
15	assign	(segid 3A4 and resid 69 and name CA)	(segid 3A4 and resid 195 and name CB)	16.71	0.88	0.89
	assign	(segid 3A4 and resid 69 and name CA)	(segid 3A4 and resid 198 and name CB)	17.66	0.97	0.97
	assign	(segid 3A4 and resid 69 and name CA)	(segid 3A4 and resid 220 and name CB)	18.88	0.61	0.61
	assign	(segid 3A4 and resid 69 and name CA)	(segid 3A4 and resid 224 and name CA)	18.42	0.61	0.61
	assign	(segid 3A4 and resid 69 and name CA)	(segid 3A4 and resid 224 and name CB)	17.33	0.64	0.65
20	assign	(segid 3A4 and resid 69 and name CA)	(segid 3A4 and resid 240 and name CA)	16.70	0.68	0.69
	assign	(segid 3A4 and resid 69 and name CA)	(segid 3A4 and resid 240 and name CB)	16.21	0.78	0.78
	assign	(segid 3A4 and resid 69 and name CA)	(segid 3A4 and resid 241 and name CA)	17.39	0.85	0.85
	assign	(segid 3A4 and resid 69 and name CA)	(segid 3A4 and resid 242 and name CA)	14.47	1.06	1.06
	assign	(segid 3A4 and resid 69 and name CA)	(segid 3A4 and resid 242 and name CB)	14.35	1.16	1.17
25	assign	(segid 3A4 and resid 69 and name CA)	(segid 3A4 and resid 243 and name CA)	12.01	0.80	0.81
	assign	(segid 3A4 and resid 69 and name CA)	(segid 3A4 and resid 243 and name CB)	12.14	0.76	0.76
	assign	(segid 3A4 and resid 69 and name CA)	(segid 3A4 and resid 244 and name CA)	14.24	0.63	0.64
	assign	(segid 3A4 and resid 69 and name CA)	(segid 3A4 and resid 244 and name CB)	15.73	0.63	0.64
	assign	(segid 3A4 and resid 69 and name CA)	(segid 3A4 and resid 245 and name CA)	14.17	0.75	0.76
30	assign	(segid 3A4 and resid 69 and name CA)	(segid 3A4 and resid 245 and name CB)	14.74	0.83	0.83
	assign	(segid 3A4 and resid 69 and name CA)	(segid 3A4 and resid 246 and name CA)	10.47	0.77	0.76
	assign	(segid 3A4 and resid 69 and name CA)	(segid 3A4 and resid 246 and name CB)	9.53	0.80	0.79
	assign	(segid 3A4 and resid 69 and name CA)	(segid 3A4 and resid 247 and name CA)	10.59	0.53	0.53
	assign	(segid 3A4 and resid 69 and name CA)	(segid 3A4 and resid 247 and name CB)	11.25	0.44	0.44
35	assign	(segid 3A4 and resid 69 and name CA)	(segid 3A4 and resid 248 and name CA)	13.75	0.63	0.62
	assign	(segid 3A4 and resid 69 and name CA)	(segid 3A4 and resid 248 and name CB)	14.97	0.64	0.64
	assign	(segid 3A4 and resid 69 and name CA)	(segid 3A4 and resid 249 and name CA)	12.51	0.82	0.81
	assign	(segid 3A4 and resid 69 and name CA)	(segid 3A4 and resid 250 and name CA)	9.89	0.76	0.76
	assign	(segid 3A4 and resid 69 and name CA)	(segid 3A4 and resid 250 and name CB)	8.70	0.73	0.73
40	assign	(segid 3A4 and resid 69 and name CA)	(segid 3A4 and resid 251 and name CA)	12.77	0.69	0.69
	assign	(segid 3A4 and resid 69 and name CA)	(segid 3A4 and resid 251 and name CB)	13.58	0.59	0.59
	assign	(segid 3A4 and resid 69 and name CA)	(segid 3A4 and resid 252 and name CA)	15.10	0.87	0.87
	assign	(segid 3A4 and resid 69 and name CA)	(segid 3A4 and resid 252 and name CB)	15.54	0.86	0.87
	assign	(segid 3A4 and resid 69 and name CA)	(segid 3A4 and resid 253 and name CA)	13.51	1.08	1.07
45	assign	(segid 3A4 and resid 69 and name CA)	(segid 3A4 and resid 254 and name CA)	12.35	1.13	1.14
	assign	(segid 3A4 and resid 69 and name CA)	(segid 3A4 and resid 255 and name CA)	15.58	1.12	1.13
	assign	(segid 3A4 and resid 69 and name CA)	(segid 3A4 and resid 256 and name CA)	18.01	0.92	0.92
	assign	(segid 3A4 and resid 69 and name CA)	(segid 3A4 and resid 257 and name CA)	18.01	0.91	0.92
	assign	(segid 3A4 and resid 69 and name CA)	(segid 3A4 and resid 258 and name CA)	17.68	0.85	0.86
50	assign	(segid 3A4 and resid 69 and name CA)	(segid 3A4 and resid 258 and name CB)	16.54	0.82	0.83
	assign	(segid 3A4 and resid 69 and name CA)	(segid 3A4 and resid 318 and name CA)	19.19	0.61	0.61
	assign	(segid 3A4 and resid 69 and name CA)	(segid 3A4 and resid 319 and name CA)	15.77	0.53	0.52
	assign	(segid 3A4 and resid 69 and name CA)	(segid 3A4 and resid 319 and name CB)	14.71	0.56	0.56
	assign	(segid 3A4 and resid 69 and name CA)	(segid 3A4 and resid 322 and name CA)	10.40	0.76	0.77
55	assign	(segid 3A4 and resid 69 and name CA)	(segid 3A4 and resid 323 and name CA)	10.33	1.14	1.13
	assign	(segid 3A4 and resid 69 and name CA)	(segid 3A4 and resid 323 and name CB)	11.16	1.23	1.24
	assign	(segid 3A4 and resid 69 and name CA)	(segid 3A4 and resid 324 and name CA)	11.70	1.21	1.21
	assign	(segid 3A4 and resid 69 and name CA)	(segid 3A4 and resid 324 and name CB)	11.07	1.23	1.22
	assign	(segid 3A4 and resid 69 and name CA)	(segid 3A4 and resid 325 and name CA)	14.68	1.34	1.34
60	assign	(segid 3A4 and resid 69 and name CA)	(segid 3A4 and resid 325 and name CB)	16.09	1.30	1.30
	assign	(segid 3A4 and resid 69 and name CA)	(segid 3A4 and resid 326 and name CA)	14.88	1.39	1.40
	assign	(segid 3A4 and resid 69 and name CA)	(segid 3A4 and resid 326 and name CB)	14.44	1.59	1.58
	assign	(segid 3A4 and resid 69 and name CA)	(segid 3A4 and resid 340 and name CA)	15.92	1.10	1.09
	assign	(segid 3A4 and resid 69 and name CA)	(segid 3A4 and resid 341 and name CA)	16.69	0.97	0.97
65	assign	(segid 3A4 and resid 69 and name CA)	(segid 3A4 and resid 342 and name CA)	14.37	0.85	0.86
	assign	(segid 3A4 and resid 69 and name CA)	(segid 3A4 and resid 343 and name CA)	15.00	0.88	0.89
	assign	(segid 3A4 and resid 69 and name CA)	(segid 3A4 and resid 343 and name CB)	15.17	0.99	1.00
	assign	(segid 3A4 and resid 69 and name CA)	(segid 3A4 and resid 344 and name CA)	14.92	0.53	0.53
	assign	(segid 3A4 and resid 69 and name CA)	(segid 3A4 and resid 344 and name CB)	15.57	0.58	0.59
70	assign	(segid 3A4 and resid 69 and name CA)	(segid 3A4 and resid 345 and name CA)	15.83	0.59	0.58
	assign	(segid 3A4 and resid 69 and name CA)	(segid 3A4 and resid 345 and name CB)	15.16	0.76	0.75
	assign	(segid 3A4 and resid 69 and name CA)	(segid 3A4 and resid 346 and name CA)	18.09	0.60	0.60
	assign	(segid 3A4 and resid 69 and name CA)	(segid 3A4 and resid 347 and name CA)	18.20	0.69	0.69
	assign	(segid 3A4 and resid 69 and name CA)	(segid 3A4 and resid 347 and name CB)	17.23	0.65	0.65
75	assign	(segid 3A4 and resid 69 and name CA)	(segid 3A4 and resid 382 and name CA)	19.21	0.46	0.45
	assign	(segid 3A4 and resid 69 and name CA)	(segid 3A4 and resid 382 and name CB)	18.81	0.50	0.51
	assign	(segid 3A4 and resid 69 and name CA)	(segid 3A4 and resid 383 and name CA)	18.55	0.46	0.45
	assign	(segid 3A4 and resid 69 and name CA)	(segid 3A4 and resid 384 and name CA)	16.12	0.37	0.37
	assign	(segid 3A4 and resid 69 and name CA)	(segid 3A4 and resid 384 and name CB)	16.78	0.37	0.36
80	assign	(segid 3A4 and resid 69 and name CA)	(segid 3A4 and resid 385 and name CA)	14.46	0.44	0.44
	assign	(segid 3A4 and resid 69 and name CA)	(segid 3A4 and resid 386 and name CA)	15.39	0.48	0.48
	assign	(segid 3A4 and resid 69 and name CA)	(segid 3A4 and resid 387 and name CA)	14.49	0.56	0.57
	assign	(segid 3A4 and resid 69 and name CA)	(segid 3A4 and resid 388 and name CA)	12.42	0.67	0.66

5	assign (segid 3A4 and resid 69 and name CA) (segid 3A4 and resid 388 and name CB) 12.11 0.96 0.96
	assign (segid 3A4 and resid 69 and name CA) (segid 3A4 and resid 389 and name CA) 9.83 0.35 0.35
	assign (segid 3A4 and resid 69 and name CA) (segid 3A4 and resid 389 and name CB) 8.84 0.46 0.47
	assign (segid 3A4 and resid 69 and name CA) (segid 3A4 and resid 390 and name CA) 12.85 0.26 0.26
	assign (segid 3A4 and resid 69 and name CA) (segid 3A4 and resid 390 and name CB) 14.21 0.21 0.21
10	assign (segid 3A4 and resid 69 and name CA) (segid 3A4 and resid 391 and name CA) 13.05 0.43 0.42
	assign (segid 3A4 and resid 69 and name CA) (segid 3A4 and resid 391 and name CB) 13.99 0.44 0.44
	assign (segid 3A4 and resid 69 and name CA) (segid 3A4 and resid 392 and name CA) 13.75 0.53 0.52
	assign (segid 3A4 and resid 69 and name CA) (segid 3A4 and resid 392 and name CB) 12.87 0.56 0.56
	assign (segid 3A4 and resid 69 and name CA) (segid 3A4 and resid 393 and name CA) 15.98 0.61 0.62
15	assign (segid 3A4 and resid 69 and name CA) (segid 3A4 and resid 394 and name CA) 18.07 0.55 0.55
	assign (segid 3A4 and resid 69 and name CA) (segid 3A4 and resid 394 and name CB) 18.03 0.49 0.48
	assign (segid 3A4 and resid 69 and name CA) (segid 3A4 and resid 69 and name C) 1.53 0.00 0.01
	assign (segid 3A4 and resid 69 and name CA) (segid 3A4 and resid 69 and name O) 2.41 0.01 0.00
	assign (segid 3A4 and resid 69 and name CA) (segid 3A4 and resid 70 and name C) 4.78 0.07 0.08
20	assign (segid 3A4 and resid 69 and name CA) (segid 3A4 and resid 70 and name CA) 3.82 0.01 0.02
	assign (segid 3A4 and resid 69 and name CA) (segid 3A4 and resid 70 and name N) 2.44 0.01 0.02
	assign (segid 3A4 and resid 69 and name CA) (segid 3A4 and resid 70 and name O) 4.89 0.13 0.13
	assign (segid 3A4 and resid 69 and name CA) (segid 3A4 and resid 71 and name CA) 7.09 0.13 0.13
	assign (segid 3A4 and resid 69 and name CA) (segid 3A4 and resid 71 and name CB) 7.91 0.26 0.27
25	assign (segid 3A4 and resid 69 and name CA) (segid 3A4 and resid 71 and name N) 5.88 0.11 0.12
	assign (segid 3A4 and resid 69 and name CA) (segid 3A4 and resid 72 and name CA) 10.08 0.27 0.28
	assign (segid 3A4 and resid 69 and name CA) (segid 3A4 and resid 73 and name CA) 12.21 0.27 0.28
	assign (segid 3A4 and resid 69 and name CA) (segid 3A4 and resid 73 and name CB) 13.38 0.53 0.53
	assign (segid 3A4 and resid 69 and name CA) (segid 3A4 and resid 74 and name CA) 10.09 0.31 0.31
30	assign (segid 3A4 and resid 69 and name CA) (segid 3A4 and resid 74 and name CB) 9.33 0.38 0.38
	assign (segid 3A4 and resid 69 and name CA) (segid 3A4 and resid 75 and name CA) 8.24 0.28 0.29
	assign (segid 3A4 and resid 69 and name CA) (segid 3A4 and resid 75 and name CB) 7.72 0.24 0.25
	assign (segid 3A4 and resid 69 and name CA) (segid 3A4 and resid 76 and name CA) 11.83 0.36 0.36
	assign (segid 3A4 and resid 69 and name CA) (segid 3A4 and resid 76 and name CB) 12.87 0.37 0.36
35	assign (segid 3A4 and resid 69 and name CA) (segid 3A4 and resid 77 and name CA) 13.24 0.36 0.37
	assign (segid 3A4 and resid 69 and name CA) (segid 3A4 and resid 77 and name CB) 13.52 0.35 0.35
	assign (segid 3A4 and resid 69 and name CA) (segid 3A4 and resid 78 and name CA) 11.17 0.44 0.43
	assign (segid 3A4 and resid 69 and name CA) (segid 3A4 and resid 78 and name CB) 9.87 0.45 0.46
	assign (segid 3A4 and resid 69 and name CA) (segid 3A4 and resid 79 and name CA) 11.46 0.44 0.43
40	assign (segid 3A4 and resid 69 and name CA) (segid 3A4 and resid 79 and name CB) 11.04 0.47 0.47
	assign (segid 3A4 and resid 69 and name CA) (segid 3A4 and resid 80 and name CA) 15.08 0.45 0.45
	assign (segid 3A4 and resid 69 and name CA) (segid 3A4 and resid 81 and name CA) 15.87 0.45 0.45
	assign (segid 3A4 and resid 69 and name CA) (segid 3A4 and resid 81 and name CB) 15.39 0.49 0.50
	assign (segid 3A4 and resid 69 and name CA) (segid 3A4 and resid 82 and name CA) 15.03 0.72 0.72
45	assign (segid 3A4 and resid 69 and name CA) (segid 3A4 and resid 82 and name CB) 13.82 0.90 0.90
	assign (segid 3A4 and resid 69 and name CA) (segid 3A4 and resid 83 and name CA) 16.36 0.28 0.29
	assign (segid 3A4 and resid 69 and name CA) (segid 3A4 and resid 83 and name CB) 16.26 0.38 0.38
	assign (segid 3A4 and resid 69 and name CA) (segid 3A4 and resid 86 and name CA) 18.72 0.44 0.44
	assign (segid 3A4 and resid 69 and name CA) (segid 3A4 and resid 86 and name CB) 17.35 0.41 0.41
50	assign (segid 3A4 and resid 69 and name N) (segid HEM and resid 1 and name CAD) 6.82 0.55 0.55
	assign (segid 3A4 and resid 69 and name N) (segid HEM and resid 1 and name CGD) 6.57 0.46 0.45
	assign (segid 3A4 and resid 69 and name N) (segid HEM and resid 1 and name O1D) 6.87 0.74 0.74
	assign (segid 3A4 and resid 69 and name N) (segid HEM and resid 1 and name O2D) 5.88 0.68 0.67
	assign (segid 3A4 and resid 69 and name N) (segid 3A4 and resid 69 and name C) 2.48 0.01 0.02
55	assign (segid 3A4 and resid 69 and name N) (segid 3A4 and resid 69 and name CA) 1.46 0.01 0.02
	assign (segid 3A4 and resid 69 and name N) (segid 3A4 and resid 69 and name O) 3.49 0.21 0.22
	assign (segid 3A4 and resid 69 and name N) (segid 3A4 and resid 70 and name C) 5.14 0.21 0.21
	assign (segid 3A4 and resid 69 and name N) (segid 3A4 and resid 70 and name CA) 4.28 0.20 0.19
	assign (segid 3A4 and resid 69 and name N) (segid 3A4 and resid 70 and name N) 2.87 0.22 0.23
60	assign (segid 3A4 and resid 69 and name N) (segid 3A4 and resid 70 and name O) 5.01 0.21 0.21
	assign (segid 3A4 and resid 69 and name N) (segid 3A4 and resid 71 and name N) 6.37 0.21 0.22
	assign (segid 3A4 and resid 69 and name N) (segid 3A4 and resid 75 and name CB) 7.34 0.24 0.24
	assign (segid 3A4 and resid 69 and name N) (segid 3A4 and resid 75 and name CG) 7.15 0.25 0.26
	assign (segid 3A4 and resid 69 and name O) (segid 3A4 and resid 70 and name C) 3.87 0.12 0.12
65	assign (segid 3A4 and resid 69 and name O) (segid 3A4 and resid 70 and name CA) 2.80 0.05 0.04
	assign (segid 3A4 and resid 69 and name O) (segid 3A4 and resid 70 and name N) 2.25 0.01 0.01
	assign (segid 3A4 and resid 69 and name O) (segid 3A4 and resid 70 and name O) 4.51 0.10 0.10
	assign (segid 3A4 and resid 69 and name O) (segid 3A4 and resid 71 and name C) 6.81 0.14 0.14
	assign (segid 3A4 and resid 69 and name O) (segid 3A4 and resid 71 and name CA) 5.88 0.24 0.23
70	assign (segid 3A4 and resid 69 and name O) (segid 3A4 and resid 71 and name CB) 6.44 0.39 0.39
	assign (segid 3A4 and resid 69 and name O) (segid 3A4 and resid 71 and name N) 4.56 0.23 0.23
	assign (segid 3A4 and resid 69 and name O) (segid 3A4 and resid 71 and name O) 6.71 0.14 0.13
	assign (segid 3A4 and resid 69 and name O) (segid 3A4 and resid 75 and name CB) 7.27 0

	assign (segid 3A4 and resid	6 and name C)	(segid 3A4 and resid	8 and name C)	4.61	0.17	0.17
	assign (segid 3A4 and resid	6 and name C)	(segid 3A4 and resid	8 and name CA)	4.46	0.14	0.13
	assign (segid 3A4 and resid	6 and name C)	(segid 3A4 and resid	8 and name CB)	5.15	0.15	0.14
	assign (segid 3A4 and resid	6 and name C)	(segid 3A4 and resid	8 and name N)	3.25	0.15	0.15
5	assign (segid 3A4 and resid	6 and name C)	(segid 3A4 and resid	8 and name O)	5.73	0.16	0.16
	assign (segid 3A4 and resid	6 and name C)	(segid 3A4 and resid	9 and name C)	4.99	0.32	0.33
	assign (segid 3A4 and resid	6 and name C)	(segid 3A4 and resid	9 and name CA)	4.64	0.27	0.28
	assign (segid 3A4 and resid	6 and name C)	(segid 3A4 and resid	9 and name CB)	4.48	0.30	0.30
	assign (segid 3A4 and resid	6 and name C)	(segid 3A4 and resid	9 and name N)	3.88	0.24	0.24
10	assign (segid 3A4 and resid	6 and name C)	(segid 3A4 and resid	9 and name O)	6.21	0.33	0.33
	assign (segid 3A4 and resid	6 and name CA)	(segid 3A4 and resid	10 and name CA)	6.41	0.37	0.36
	assign (segid 3A4 and resid	6 and name CA)	(segid 3A4 and resid	10 and name CB)	6.14	0.32	0.32
	assign (segid 3A4 and resid	6 and name CA)	(segid 3A4 and resid	10 and name N)	5.38	0.38	0.37
	assign (segid 3A4 and resid	6 and name CA)	(segid 3A4 and resid	11 and name CA)	8.71	0.21	0.20
15	assign (segid 3A4 and resid	6 and name CA)	(segid 3A4 and resid	11 and name CB)	8.69	0.15	0.15
	assign (segid 3A4 and resid	6 and name CA)	(segid 3A4 and resid	12 and name CA)	10.10	0.30	0.31
	assign (segid 3A4 and resid	6 and name CA)	(segid 3A4 and resid	12 and name CB)	9.72	0.34	0.35
	assign (segid 3A4 and resid	6 and name CA)	(segid 3A4 and resid	13 and name CA)	11.10	0.62	0.63
	assign (segid 3A4 and resid	6 and name CA)	(segid 3A4 and resid	13 and name CB)	10.41	0.72	0.72
20	assign (segid 3A4 and resid	6 and name CA)	(segid 3A4 and resid	19 and name CA)	16.26	1.52	1.53
	assign (segid 3A4 and resid	6 and name CA)	(segid 3A4 and resid	21 and name CA)	16.18	1.29	1.29
	assign (segid 3A4 and resid	6 and name CA)	(segid 3A4 and resid	21 and name CB)	15.24	1.30	1.30
	assign (segid 3A4 and resid	6 and name CA)	(segid 3A4 and resid	23 and name CA)	14.57	1.64	1.64
	assign (segid 3A4 and resid	6 and name CA)	(segid 3A4 and resid	23 and name CB)	13.20	1.65	1.65
25	assign (segid 3A4 and resid	6 and name CA)	(segid 3A4 and resid	25 and name CA)	15.43	1.91	1.92
	assign (segid 3A4 and resid	6 and name CA)	(segid 3A4 and resid	26 and name CA)	17.70	1.36	1.35
	assign (segid 3A4 and resid	6 and name CA)	(segid 3A4 and resid	30 and name CA)	17.12	1.91	1.90
	assign (segid 3A4 and resid	6 and name CA)	(segid 3A4 and resid	313 and name CA)	17.46	1.55	1.54
	assign (segid 3A4 and resid	6 and name CA)	(segid 3A4 and resid	314 and name CA)	16.32	1.52	1.52
30	assign (segid 3A4 and resid	6 and name CA)	(segid 3A4 and resid	315 and name CA)	14.26	1.86	1.86
	assign (segid 3A4 and resid	6 and name CA)	(segid 3A4 and resid	315 and name CB)	15.04	1.97	1.97
	assign (segid 3A4 and resid	6 and name CA)	(segid 3A4 and resid	316 and name CA)	12.79	1.93	1.93
	assign (segid 3A4 and resid	6 and name CA)	(segid 3A4 and resid	317 and name CA)	12.79	1.36	1.37
	assign (segid 3A4 and resid	6 and name CA)	(segid 3A4 and resid	318 and name CA)	13.08	1.87	1.87
35	assign (segid 3A4 and resid	6 and name CA)	(segid 3A4 and resid	318 and name CB)	14.20	2.17	2.17
	assign (segid 3A4 and resid	6 and name CA)	(segid 3A4 and resid	319 and name CA)	13.38	1.64	1.64
	assign (segid 3A4 and resid	6 and name CA)	(segid 3A4 and resid	319 and name CB)	14.66	1.70	1.70
	assign (segid 3A4 and resid	6 and name CA)	(segid 3A4 and resid	31 and name CA)	16.73	1.46	1.47
	assign (segid 3A4 and resid	6 and name CA)	(segid 3A4 and resid	32 and name CA)	13.80	1.21	1.20
40	assign (segid 3A4 and resid	6 and name CA)	(segid 3A4 and resid	32 and name CB)	12.50	1.22	1.23
	assign (segid 3A4 and resid	6 and name CA)	(segid 3A4 and resid	33 and name CA)	15.07	0.97	0.96
	assign (segid 3A4 and resid	6 and name CA)	(segid 3A4 and resid	33 and name CB)	16.14	0.89	0.88
	assign (segid 3A4 and resid	6 and name CA)	(segid 3A4 and resid	343 and name CA)	17.92	1.60	1.60
	assign (segid 3A4 and resid	6 and name CA)	(segid 3A4 and resid	344 and name CA)	14.68	1.56	1.56
45	assign (segid 3A4 and resid	6 and name CA)	(segid 3A4 and resid	344 and name CB)	13.54	1.66	1.66
	assign (segid 3A4 and resid	6 and name CA)	(segid 3A4 and resid	345 and name CA)	14.65	1.19	1.20
	assign (segid 3A4 and resid	6 and name CA)	(segid 3A4 and resid	345 and name CB)	15.91	1.19	1.18
	assign (segid 3A4 and resid	6 and name CA)	(segid 3A4 and resid	346 and name CA)	11.63	0.82	0.83
	assign (segid 3A4 and resid	6 and name CA)	(segid 3A4 and resid	346 and name CB)	10.70	0.62	0.62
50	assign (segid 3A4 and resid	6 and name CA)	(segid 3A4 and resid	347 and name CA)	13.26	0.64	0.63
	assign (segid 3A4 and resid	6 and name CA)	(segid 3A4 and resid	347 and name CB)	13.90	0.81	0.80
	assign (segid 3A4 and resid	6 and name CA)	(segid 3A4 and resid	348 and name CA)	10.74	0.93	0.94
	assign (segid 3A4 and resid	6 and name CA)	(segid 3A4 and resid	349 and name CA)	10.85	1.38	1.38
	assign (segid 3A4 and resid	6 and name CA)	(segid 3A4 and resid	349 and name CB)	10.70	1.29	1.29
55	assign (segid 3A4 and resid	6 and name CA)	(segid 3A4 and resid	34 and name CA)	13.30	1.22	1.22
	assign (segid 3A4 and resid	6 and name CA)	(segid 3A4 and resid	34 and name CB)	12.63	1.49	1.49
	assign (segid 3A4 and resid	6 and name CA)	(segid 3A4 and resid	350 and name CA)	14.34	1.16	1.16
	assign (segid 3A4 and resid	6 and name CA)	(segid 3A4 and resid	350 and name CB)	15.14	0.91	0.91
60	assign (segid 3A4 and resid	6 and name CA)	(segid 3A4 and resid	351 and name CA)	14.67	1.35	1.35
	assign (segid 3A4 and resid	6 and name CA)	(segid 3A4 and resid	352 and name CA)	13.25	2.02	2.02
	assign (segid 3A4 and resid	6 and name CA)	(segid 3A4 and resid	352 and name CB)	11.87	2.12	2.12
	assign (segid 3A4 and resid	6 and name CA)	(segid 3A4 and resid	35 and name CA)	16.12	1.34	1.34
	assign (segid 3A4 and resid	6 and name CA)	(segid 3A4 and resid	361 and name CA)	14.19	2.70	2.70
	assign (segid 3A4 and resid	6 and name CA)	(segid 3A4 and resid	361 and name CB)	13.60	2.85	2.85
65	assign (segid 3A4 and resid	6 and name CA)	(segid 3A4 and resid	382 and name CA)	18.25	0.86	0.86
	assign (segid 3A4 and resid	6 and name CA)	(segid 3A4 and resid	382 and name CB)	17.85	0.76	0.76
	assign (segid 3A4 and resid	6 and name CA)	(segid 3A4 and resid	383 and name CA)	17.04	1.03	1.03
	assign (segid 3A4 and resid	6 and name CA)	(segid 3A4 and resid	39 and name CB)	17.29	0.92	0.92
70	assign (segid 3A4 and resid	6 and name CA)	(segid 3A4 and resid	424 and name CA)	17.12	1.99	1.98
	assign (segid 3A4 and resid	6 and name CA)	(segid 3A4 and resid	425 and name CA)	15.16	2.23	2.23
	assign (segid 3A4 and resid	6 and name CA)	(segid 3A4 and resid	426 and name CA)	12.54	2.01	2.01
	assign (segid 3A4 and resid	6 and name CA)	(segid 3A4 and resid	427 and name CA)	11.63	2.63	2.63
	assign (segid 3A4 and resid	6 and name CA)	(segid 3A4 and resid	428 and name CA)	10.47	2.09	2.09
	assign (segid 3A4 and resid	6 and name CA)	(segid 3A4 and resid	429 and name CA)	9.87	1.70	1.70
75	assign (segid 3A4 and resid	6 and name CA)	(segid 3A4 and resid	430 and name CA)	10.15	0.86	0.87
	assign (segid 3A4 and resid	6 and name CA)	(segid 3A4 and resid	431 and name CA)	12.20	1.47	1.46
	assign (segid 3A4 and resid	6 and name CA)	(segid 3A4 and resid	433 and name CA)	11.14	1.62	1.62
	assign (segid 3A4 and resid	6 and name CA)	(segid 3A4 and resid	434 and name CA)	13.17	2.15	2.15
80	assign (segid 3A4 and resid	6 and name CA)	(segid 3A4 and resid	435 and name CA)	14.98	2.56	2.56
	assign (segid 3A4 and resid	6 and name C)	(segid 3A4 and resid	6 and name C)	1.52	0.01	0.01
	assign (segid 3A4 and resid	6 and name CA)	(segid 3A4 and resid	6 and name CB)	1.55	0.02	0.03
	assign (segid 3A4 and resid	6 and name O)	(segid 3A4 and resid	6 and name O)	2.39	0.01	0.02
	assign (segid 3A4 and resid	6 and name CA)	(segid 3A4 and resid	7 and name C)	4.45	0.06	0.07

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	assign (segid 3A4 and resid 6 and name CB) (segid 3A4 and resid 9 and name C)	6.89	0.37	0.38
	assign (segid 3A4 and resid 6 and name CB) (segid 3A4 and resid 9 and name CA)	6.50	0.35	0.36
	assign (segid 3A4 and resid 6 and name CB) (segid 3A4 and resid 9 and name CB)	5.80	0.44	0.44
	assign (segid 3A4 and resid 6 and name CB) (segid 3A4 and resid 9 and name N)	6.05	0.28	0.28
5	assign (segid 3A4 and resid 6 and name N) (segid 3A4 and resid 10 and name N)	6.45	0.38	0.38
	assign (segid 3A4 and resid 6 and name N) (segid 3A4 and resid 6 and name C)	2.50	0.02	0.02
	assign (segid 3A4 and resid 6 and name N) (segid 3A4 and resid 6 and name CA)	1.46	0.01	0.01
	assign (segid 3A4 and resid 6 and name N) (segid 3A4 and resid 6 and name CB)	2.43	0.04	0.05
	assign (segid 3A4 and resid 6 and name N) (segid 3A4 and resid 6 and name O)	3.55	0.04	0.04
10	assign (segid 3A4 and resid 6 and name N) (segid 3A4 and resid 7 and name C)	4.88	0.10	0.09
	assign (segid 3A4 and resid 6 and name N) (segid 3A4 and resid 7 and name CA)	4.30	0.06	0.07
	assign (segid 3A4 and resid 6 and name N) (segid 3A4 and resid 7 and name CB)	5.10	0.12	0.13
	assign (segid 3A4 and resid 6 and name N) (segid 3A4 and resid 7 and name N)	2.89	0.07	0.07
	assign (segid 3A4 and resid 6 and name N) (segid 3A4 and resid 7 and name O)	5.98	0.13	0.12
15	assign (segid 3A4 and resid 6 and name N) (segid 3A4 and resid 8 and name C)	5.92	0.31	0.31
	assign (segid 3A4 and resid 6 and name N) (segid 3A4 and resid 8 and name CA)	5.54	0.24	0.23
	assign (segid 3A4 and resid 6 and name N) (segid 3A4 and resid 8 and name CB)	5.56	0.28	0.27
	assign (segid 3A4 and resid 6 and name N) (segid 3A4 and resid 8 and name N)	4.49	0.19	0.19
	assign (segid 3A4 and resid 6 and name N) (segid 3A4 and resid 8 and name O)	7.14	0.30	0.30
20	assign (segid 3A4 and resid 6 and name N) (segid 3A4 and resid 9 and name C)	6.82	0.44	0.44
	assign (segid 3A4 and resid 6 and name N) (segid 3A4 and resid 9 and name CA)	6.00	0.47	0.47
	assign (segid 3A4 and resid 6 and name N) (segid 3A4 and resid 9 and name CB)	5.50	0.53	0.54
	assign (segid 3A4 and resid 6 and name N) (segid 3A4 and resid 9 and name N)	5.18	0.39	0.39
	assign (segid 3A4 and resid 6 and name N) (segid 3A4 and resid 10 and name C)	5.17	0.32	0.32
25	assign (segid 3A4 and resid 6 and name O) (segid 3A4 and resid 10 and name CA)	4.08	0.35	0.34
	assign (segid 3A4 and resid 6 and name O) (segid 3A4 and resid 10 and name CB)	3.88	0.29	0.30
	assign (segid 3A4 and resid 6 and name O) (segid 3A4 and resid 10 and name N)	3.12	0.35	0.35
	assign (segid 3A4 and resid 6 and name O) (segid 3A4 and resid 10 and name O)	6.32	0.32	0.33
	assign (segid 3A4 and resid 6 and name O) (segid 3A4 and resid 11 and name C)	7.32	0.27	0.26
30	assign (segid 3A4 and resid 6 and name O) (segid 3A4 and resid 11 and name CA)	6.46	0.24	0.24
	assign (segid 3A4 and resid 6 and name O) (segid 3A4 and resid 11 and name CB)	6.63	0.20	0.19
	assign (segid 3A4 and resid 6 and name O) (segid 3A4 and resid 11 and name N)	5.13	0.26	0.26
	assign (segid 3A4 and resid 6 and name O) (segid 3A4 and resid 12 and name N)	6.97	0.28	0.28
35	assign (segid 3A4 and resid 6 and name O) (segid 3A4 and resid 6 and name CB)	3.32	0.11	0.11
	assign (segid 3A4 and resid 6 and name O) (segid 3A4 and resid 7 and name C)	2.94	0.08	0.07
	assign (segid 3A4 and resid 6 and name O) (segid 3A4 and resid 7 and name CA)	2.71	0.05	0.05
	assign (segid 3A4 and resid 6 and name O) (segid 3A4 and resid 7 and name CB)	4.21	0.05	0.05
	assign (segid 3A4 and resid 6 and name O) (segid 3A4 and resid 7 and name N)	2.22	0.02	0.02
	assign (segid 3A4 and resid 6 and name O) (segid 3A4 and resid 7 and name O)	3.50	0.20	0.20
40	assign (segid 3A4 and resid 6 and name O) (segid 3A4 and resid 8 and name C)	4.07	0.17	0.17
	assign (segid 3A4 and resid 6 and name O) (segid 3A4 and resid 8 and name CA)	4.27	0.11	0.12
	assign (segid 3A4 and resid 6 and name O) (segid 3A4 and resid 8 and name CB)	5.19	0.14	0.15
	assign (segid 3A4 and resid 6 and name O) (segid 3A4 and resid 8 and name N)	3.30	0.13	0.13
	assign (segid 3A4 and resid 6 and name O) (segid 3A4 and resid 8 and name O)	5.07	0.17	0.16
45	assign (segid 3A4 and resid 6 and name O) (segid 3A4 and resid 9 and name C)	3.88	0.34	0.33
	assign (segid 3A4 and resid 6 and name O) (segid 3A4 and resid 9 and name CA)	3.75	0.25	0.24
	assign (segid 3A4 and resid 6 and name O) (segid 3A4 and resid 9 and name CB)	3.67	0.21	0.21
	assign (segid 3A4 and resid 6 and name O) (segid 3A4 and resid 9 and name N)	3.22	0.20	0.21
	assign (segid 3A4 and resid 6 and name O) (segid 3A4 and resid 9 and name O)	5.07	0.35	0.35
50	assign (segid 3A4 and resid 70 and name C) (segid 3A4 and resid 70 and name O)	1.23	0.00	0.01
	assign (segid 3A4 and resid 70 and name C) (segid 3A4 and resid 71 and name C)	3.30	0.07	0.06
	assign (segid 3A4 and resid 70 and name C) (segid 3A4 and resid 71 and name CA)	2.47	0.03	0.03
	assign (segid 3A4 and resid 70 and name C) (segid 3A4 and resid 71 and name CB)	3.65	0.07	0.07
	assign (segid 3A4 and resid 70 and name C) (segid 3A4 and resid 71 and name CG)	4.09	0.24	0.25
55	assign (segid 3A4 and resid 70 and name C) (segid 3A4 and resid 71 and name N)	1.34	0.02	0.01
	assign (segid 3A4 and resid 70 and name C) (segid 3A4 and resid 71 and name O)	3.48	0.12	0.11
	assign (segid 3A4 and resid 70 and name C) (segid 3A4 and resid 72 and name C)	6.18	0.11	0.10
	assign (segid 3A4 and resid 70 and name C) (segid 3A4 and resid 72 and name CA)	5.48	0.13	0.14
	assign (segid 3A4 and resid 70 and name C) (segid 3A4 and resid 72 and name N)	4.33	0.12	0.11
60	assign (segid 3A4 and resid 70 and name C) (segid 3A4 and resid 72 and name O)	6.42	0.20	0.20
	assign (segid 3A4 and resid 70 and name C) (segid 3A4 and resid 74 and name C)	6.18	0.57	0.57
	assign (segid 3A4 and resid 70 and name C) (segid 3A4 and resid 75 and name C)	6.47	0.45	0.46
	assign (segid 3A4 and resid 70 and name C) (segid 3A4 and resid 75 and name CA)	5.05	0.48	0.49
	assign (segid 3A4 and resid 70 and name C) (segid 3A4 and resid 75 and name CB)	4.19	0.39	0.39
65	assign (segid 3A4 and resid 70 and name C) (segid 3A4 and resid 75 and name CG)	4.79	0.39	0.38
	assign (segid 3A4 and resid 70 and name C) (segid 3A4 and resid 75 and name N)	5.15	0.56	0.55
	assign (segid 3A4 and resid 70 and name CA) (segid 3A4 and resid 224 and name CA)	17.98	0.58	0.59
	assign (segid 3A4 and resid 70 and name CA) (segid 3A4 and resid 224 and name CB)	17.11	0.61	0.61
	assign (segid 3A4 and resid 70 and name CA) (segid 3A4 and resid 240 and name CA)	15.69	0.74	0.74
70	assign (segid 3A4 and resid 70 and name CA) (segid 3A4 and resid 240 and name CB)	15.13	0.88	0.87
	assign (segid 3A4 and resid 70 and name CA) (segid 3A4 and resid 241 and name CA)	17.14	0.84	0.85
	assign (segid 3A4 and resid 70 and name CA) (segid 3A4 and resid 242 and name CA)	14.57	1.09	1.09
	assign (segid 3A4 and resid 70 and name CA) (segid 3A4 and resid 242 and name CB)	14.33	1.20	1.20
75	assign (segid 3A4 and resid 70 and name CA) (segid 3A4 and resid 243 and name CA)	11.73	0.91	0.91
	assign (segid 3A4 and resid 70 and name CA) (segid 3A4 and resid 243 and name CB)	11.40	0.89	0.88
	assign (segid 3A4 and resid 70 and name CA) (segid 3A4 and resid 244 and name CA)	14.33	0.69	0.69
	assign (segid 3A4 and resid 70 and name CA) (segid 3A4 and resid 244 and name CB)	15.73	0.68	0.68
	assign (segid 3A4 and resid 70 and name CA) (segid 3A4 and resid 245 and name CA)	15.13	0.80	0.80
80	assign (segid 3A4 and resid 70 and name CA) (segid 3A4 and resid 245 and name CB)	15.73	0.89	0.89
	assign (segid 3A4 and resid 70 and name CA) (segid 3A4 and resid 246 and name CA)	11.75	0.82	0.81
	assign (segid 3A4 and resid 70 and name CA) (segid 3A4 and resid 246 and name CB)	10.60	0.86	0.85
	assign (segid 3A4 and resid 70 and name CA) (segid 3A4 and resid 247 and name CA)	11.57	0.45	0.45
	assign (segid 3A4 and resid 70 and name CA) (segid 3A4 and resid 247 and name CB)	11.79	0.34	0.34

5	assign (segid 3A4 and resid 70 and name CA) (segid 3A4 and resid 248 and name CA)	15.18	0.48	0.48
	assign (segid 3A4 and resid 70 and name CA) (segid 3A4 and resid 248 and name CB)	16.32	0.53	0.52
	assign (segid 3A4 and resid 70 and name CA) (segid 3A4 and resid 249 and name CA)	14.72	0.74	0.74
	assign (segid 3A4 and resid 70 and name CA) (segid 3A4 and resid 250 and name CA)	12.27	0.64	0.64
	assign (segid 3A4 and resid 70 and name CA) (segid 3A4 and resid 250 and name CB)	10.88	0.61	0.60
	assign (segid 3A4 and resid 70 and name CA) (segid 3A4 and resid 251 and name CA)	14.74	0.43	0.43
	assign (segid 3A4 and resid 70 and name CA) (segid 3A4 and resid 251 and name CB)	15.25	0.31	0.31
	assign (segid 3A4 and resid 70 and name CA) (segid 3A4 and resid 252 and name CA)	17.55	0.62	0.62
	assign (segid 3A4 and resid 70 and name CA) (segid 3A4 and resid 252 and name CB)	18.00	0.64	0.64
10	assign (segid 3A4 and resid 70 and name CA) (segid 3A4 and resid 253 and name CA)	16.50	0.88	0.88
	assign (segid 3A4 and resid 70 and name CA) (segid 3A4 and resid 254 and name CA)	15.17	0.86	0.86
	assign (segid 3A4 and resid 70 and name CA) (segid 3A4 and resid 255 and name CA)	18.11	0.84	0.83
	assign (segid 3A4 and resid 70 and name CA) (segid 3A4 and resid 319 and name CA)	18.64	0.55	0.54
	assign (segid 3A4 and resid 70 and name CA) (segid 3A4 and resid 319 and name CB)	17.46	0.54	0.55
15	assign (segid 3A4 and resid 70 and name CA) (segid 3A4 and resid 322 and name CA)	12.42	0.48	0.47
	assign (segid 3A4 and resid 70 and name CA) (segid 3A4 and resid 323 and name CA)	11.35	0.73	0.73
	assign (segid 3A4 and resid 70 and name CA) (segid 3A4 and resid 323 and name CB)	11.92	0.91	0.91
	assign (segid 3A4 and resid 70 and name CA) (segid 3A4 and resid 324 and name CA)	12.07	0.90	0.89
	assign (segid 3A4 and resid 70 and name CA) (segid 3A4 and resid 324 and name CB)	11.41	0.92	0.93
20	assign (segid 3A4 and resid 70 and name CA) (segid 3A4 and resid 325 and name CA)	14.29	1.11	1.11
	assign (segid 3A4 and resid 70 and name CA) (segid 3A4 and resid 325 and name CB)	15.77	1.08	1.07
	assign (segid 3A4 and resid 70 and name CA) (segid 3A4 and resid 326 and name CA)	13.64	1.21	1.21
	assign (segid 3A4 and resid 70 and name CA) (segid 3A4 and resid 326 and name CB)	12.91	1.39	1.39
	assign (segid 3A4 and resid 70 and name CA) (segid 3A4 and resid 339 and name CA)	17.80	1.25	1.24
25	assign (segid 3A4 and resid 70 and name CA) (segid 3A4 and resid 339 and name CB)	18.06	1.33	1.32
	assign (segid 3A4 and resid 70 and name CA) (segid 3A4 and resid 340 and name CA)	15.75	1.34	1.34
	assign (segid 3A4 and resid 70 and name CA) (segid 3A4 and resid 341 and name CA)	17.15	1.06	1.06
	assign (segid 3A4 and resid 70 and name CA) (segid 3A4 and resid 341 and name CB)	18.24	1.01	1.00
30	assign (segid 3A4 and resid 70 and name CA) (segid 3A4 and resid 342 and name CA)	15.50	0.86	0.86
	assign (segid 3A4 and resid 70 and name CA) (segid 3A4 and resid 343 and name CA)	16.26	0.72	0.72
	assign (segid 3A4 and resid 70 and name CA) (segid 3A4 and resid 343 and name CB)	16.15	0.82	0.82
	assign (segid 3A4 and resid 70 and name CA) (segid 3A4 and resid 344 and name CA)	16.81	0.37	0.37
	assign (segid 3A4 and resid 70 and name CA) (segid 3A4 and resid 344 and name CB)	17.67	0.55	0.56
35	assign (segid 3A4 and resid 70 and name CA) (segid 3A4 and resid 345 and name CA)	17.51	0.55	0.54
	assign (segid 3A4 and resid 70 and name CA) (segid 3A4 and resid 345 and name CB)	16.66	0.78	0.77
	assign (segid 3A4 and resid 70 and name CA) (segid 3A4 and resid 384 and name CA)	17.66	0.49	0.49
	assign (segid 3A4 and resid 70 and name CA) (segid 3A4 and resid 384 and name CB)	18.13	0.48	0.49
	assign (segid 3A4 and resid 70 and name CA) (segid 3A4 and resid 385 and name CA)	15.68	0.73	0.73
	assign (segid 3A4 and resid 70 and name CA) (segid 3A4 and resid 386 and name CA)	15.74	0.89	0.89
40	assign (segid 3A4 and resid 70 and name CA) (segid 3A4 and resid 387 and name CA)	14.00	0.80	0.80
	assign (segid 3A4 and resid 70 and name CA) (segid 3A4 and resid 388 and name CA)	11.35	1.09	1.09
	assign (segid 3A4 and resid 70 and name CA) (segid 3A4 and resid 388 and name CB)	10.65	1.36	1.37
	assign (segid 3A4 and resid 70 and name CA) (segid 3A4 and resid 389 and name CA)	9.76	0.59	0.59
45	assign (segid 3A4 and resid 70 and name CA) (segid 3A4 and resid 389 and name CB)	9.02	0.58	0.58
	assign (segid 3A4 and resid 70 and name CA) (segid 3A4 and resid 390 and name CA)	13.29	0.45	0.45
	assign (segid 3A4 and resid 70 and name CA) (segid 3A4 and resid 390 and name CB)	14.43	0.53	0.53
	assign (segid 3A4 and resid 70 and name CA) (segid 3A4 and resid 391 and name CA)	14.16	0.36	0.36
	assign (segid 3A4 and resid 70 and name CA) (segid 3A4 and resid 391 and name CB)	15.36	0.39	0.39
	assign (segid 3A4 and resid 70 and name CA) (segid 3A4 and resid 392 and name CA)	14.36	0.39	0.39
50	assign (segid 3A4 and resid 70 and name CA) (segid 3A4 and resid 392 and name CB)	13.40	0.39	0.40
	assign (segid 3A4 and resid 70 and name CA) (segid 3A4 and resid 393 and name CA)	17.21	0.45	0.45
	assign (segid 3A4 and resid 70 and name CA) (segid 3A4 and resid 394 and name CA)	19.26	0.35	0.35
	assign (segid 3A4 and resid 70 and name CA) (segid 3A4 and resid 394 and name CB)	19.04	0.33	0.33
55	assign (segid 3A4 and resid 70 and name CA) (segid 3A4			

	assign (segid 3A4 and resid 70 and name CA) (segid 3A4 and resid 80 and name CA)	13.35	0.58	0.58
	assign (segid 3A4 and resid 70 and name CA) (segid 3A4 and resid 81 and name CA)	14.54	0.59	0.60
	assign (segid 3A4 and resid 70 and name CA) (segid 3A4 and resid 81 and name CB)	14.06	0.66	0.66
	assign (segid 3A4 and resid 70 and name CA) (segid 3A4 and resid 82 and name CA)	14.54	0.52	0.52
5	assign (segid 3A4 and resid 70 and name CA) (segid 3A4 and resid 82 and name CB)	13.57	0.68	0.68
	assign (segid 3A4 and resid 70 and name CA) (segid 3A4 and resid 83 and name CA)	15.74	0.41	0.41
	assign (segid 3A4 and resid 70 and name CA) (segid 3A4 and resid 83 and name CB)	15.38	0.52	0.53
	assign (segid 3A4 and resid 70 and name CA) (segid 3A4 and resid 84 and name CA)	18.95	0.48	0.49
	assign (segid 3A4 and resid 70 and name CA) (segid 3A4 and resid 86 and name CB)	17.72	0.50	0.50
10	assign (segid 3A4 and resid 70 and name N) (segid HEM and resid 1 and name O2D)	6.92	0.32	0.32
	assign (segid 3A4 and resid 70 and name N) (segid 3A4 and resid 70 and name C)	2.51	0.05	0.05
	assign (segid 3A4 and resid 70 and name N) (segid 3A4 and resid 70 and name CA)	1.45	0.01	0.01
	assign (segid 3A4 and resid 70 and name N) (segid 3A4 and resid 70 and name O)	2.86	0.08	0.09
	assign (segid 3A4 and resid 70 and name N) (segid 3A4 and resid 71 and name C)	5.75	0.07	0.07
15	assign (segid 3A4 and resid 70 and name N) (segid 3A4 and resid 71 and name CA)	4.94	0.07	0.07
	assign (segid 3A4 and resid 70 and name N) (segid 3A4 and resid 71 and name CB)	5.92	0.13	0.14
	assign (segid 3A4 and resid 70 and name N) (segid 3A4 and resid 71 and name CG)	5.97	0.31	0.31
	assign (segid 3A4 and resid 70 and name N) (segid 3A4 and resid 71 and name N)	3.65	0.05	0.06
	assign (segid 3A4 and resid 70 and name N) (segid 3A4 and resid 71 and name O)	5.71	0.14	0.13
20	assign (segid 3A4 and resid 70 and name N) (segid 3A4 and resid 72 and name CA)	7.84	0.16	0.16
	assign (segid 3A4 and resid 70 and name N) (segid 3A4 and resid 72 and name N)	6.78	0.12	0.12
	assign (segid 3A4 and resid 70 and name N) (segid 3A4 and resid 74 and name C)	7.29	0.39	0.40
	assign (segid 3A4 and resid 70 and name N) (segid 3A4 and resid 75 and name CA)	6.19	0.40	0.39
	assign (segid 3A4 and resid 70 and name N) (segid 3A4 and resid 75 and name CB)	5.64	0.28	0.28
25	assign (segid 3A4 and resid 70 and name N) (segid 3A4 and resid 75 and name CG)	5.93	0.32	0.33
	assign (segid 3A4 and resid 70 and name N) (segid 3A4 and resid 75 and name N)	6.50	0.39	0.38
	assign (segid 3A4 and resid 70 and name O) (segid HEM and resid 1 and name O2D)	6.48	0.43	0.43
	assign (segid 3A4 and resid 70 and name O) (segid 3A4 and resid 71 and name C)	3.55	0.16	0.16
	assign (segid 3A4 and resid 70 and name O) (segid 3A4 and resid 71 and name CA)	2.82	0.03	0.04
30	assign (segid 3A4 and resid 70 and name O) (segid 3A4 and resid 71 and name CB)	4.16	0.11	0.10
	assign (segid 3A4 and resid 70 and name O) (segid 3A4 and resid 71 and name CG)	4.53	0.32	0.32
	assign (segid 3A4 and resid 70 and name O) (segid 3A4 and resid 71 and name N)	2.26	0.03	0.02
	assign (segid 3A4 and resid 70 and name O) (segid 3A4 and resid 71 and name O)	3.95	0.15	0.16
	assign (segid 3A4 and resid 70 and name O) (segid 3A4 and resid 72 and name C)	6.37	0.26	0.27
35	assign (segid 3A4 and resid 70 and name O) (segid 3A4 and resid 72 and name CA)	5.43	0.31	0.30
	assign (segid 3A4 and resid 70 and name O) (segid 3A4 and resid 72 and name N)	4.28	0.25	0.24
	assign (segid 3A4 and resid 70 and name O) (segid 3A4 and resid 72 and name O)	6.69	0.08	0.08
	assign (segid 3A4 and resid 70 and name O) (segid 3A4 and resid 75 and name C)	6.28	0.54	0.54
	assign (segid 3A4 and resid 70 and name O) (segid 3A4 and resid 75 and name CA)	4.99	0.56	0.57
40	assign (segid 3A4 and resid 70 and name O) (segid 3A4 and resid 75 and name CB)	3.88	0.53	0.53
	assign (segid 3A4 and resid 70 and name O) (segid 3A4 and resid 75 and name CG)	4.12	0.50	0.51
	assign (segid 3A4 and resid 70 and name O) (segid 3A4 and resid 75 and name N)	5.39	0.62	0.62
	assign (segid 3A4 and resid 71 and name C) (segid 3A4 and resid 71 and name CB)	2.49	0.03	0.02
	assign (segid 3A4 and resid 71 and name C) (segid 3A4 and resid 71 and name CG)	3.98	0.21	0.21
45	assign (segid 3A4 and resid 71 and name C) (segid 3A4 and resid 71 and name O)	1.24	0.01	0.01
	assign (segid 3A4 and resid 71 and name C) (segid 3A4 and resid 72 and name C)	2.97	0.05	0.06
	assign (segid 3A4 and resid 71 and name C) (segid 3A4 and resid 72 and name CA)	2.44	0.02	0.01
	assign (segid 3A4 and resid 71 and name C) (segid 3A4 and resid 72 and name N)	1.33	0.02	0.01
	assign (segid 3A4 and resid 71 and name C) (segid 3A4 and resid 72 and name O)	3.35	0.34	0.34
50	assign (segid 3A4 and resid 71 and name C) (segid 3A4 and resid 73 and name CA)	5.18	1.03	1.04
	assign (segid 3A4 and resid 71 and name C) (segid 3A4 and resid 73 and name N)	4.33	1.01	1.00
	assign (segid 3A4 and resid 71 and name C) (segid 3A4 and resid 74 and name C)	5.32	0.84	0.84
	assign (segid 3A4 and resid 71 and name C) (segid 3A4 and resid 74 and name N)	4.82	1.17	1.17
	assign (segid 3A4 and resid 71 and name C) (segid 3A4 and resid 75 and name C)	5.78	0.41	0.40
	assign (segid 3A4 and resid 71 and name C) (segid 3A4 and resid 75 and name CA)	4.65	0.46	0.47
55	assign (segid 3A4 and resid 71 and name C) (segid 3A4 and resid 75 and name CB)	3.78	0.24	0.24
	assign (segid 3A4 and resid 71 and name C) (segid 3A4 and resid 75 and name CG)	4.78	0.16	0.16
	assign (segid 3A4 and resid 71 and name C) (segid 3A4 and resid 75 and name N)	4.24	0.75	0.76
	assign (segid 3A4 and resid 71 and name C) (segid 3A4 and resid 75 and name O)	6.85	0.36	0.37
60	assign (segid 3A4 and resid 71 and name C) (segid 3A4 and resid 76 and name N)	5.83	0.44	0.45
	assign (segid 3A4 and resid 71 and name CA) (segid 3A4 and resid 240 and name CB)	17.27	1.30	1.30
	assign (segid 3A4 and resid 71 and name CA) (segid 3A4 and resid 243 and name CA)	14.56	1.19	1.19
	assign (segid 3A4 and resid 71 and name CA) (segid 3A4 and resid 243 and name CB)	13.95	1.19	1.20
	assign (segid 3A4 and resid 71 and name CA) (segid 3A4 and resid 244 and name CA)	17.18	0.96	0.96
65	assign (segid 3A4 and resid 71 and name CA) (segid 3A4 and resid 246 and name CA)	15.22	0.99	0.99
	assign (segid 3A4 and resid 71 and name CA) (segid 3A4 and resid 246 and name CB)	14.06	1.05	1.05
	assign (segid 3A4 and resid 71 and name CA) (segid 3A4 and resid 247 and name CA)	14.72	0.64	0.64
	assign (segid 3A4 and resid 71 and name CA) (segid 3A4 and resid 247 and name CB)	14.71	0.58	0.58
70	assign (segid 3A4 and resid 71 and name CA) (segid 3A4 and resid 248 and name CA)	18.39	0.60	0.61
	assign (segid 3A4 and resid 71 and name CA) (segid 3A4 and resid 249 and name CA)	18.22	0.81	0.81
	assign (segid 3A4 and resid 71 and name CA) (segid 3A4 and resid 250 and name CA)	15.59	0.64	0.65
	assign (segid 3A4 and resid 71 and name CA) (segid 3A4 and resid 250 and name CB)	14.17	0.63	0.62
	assign (segid 3A4 and resid 71 and name CA) (segid 3A4 and resid 251 and name CA)	17.70	0.39	0.39
	assign (segid 3A4 and resid 71 and name CA) (segid 3A4 and resid 251 and name CB)	18.13	0.32	0.32
75	assign (segid 3A4 and resid 71 and name CA) (segid 3A4 and resid 254 and name CA)	17.98	0.75	0.75
	assign (segid 3A4 and resid 71 and name CA) (segid 3A4 and resid 322 and name CA)	12.85	0.48	0.48
	assign (segid 3A4 and resid 71 and name CA) (segid 3A4 and resid 323 and name CA)	10.91	0.34	0.34
	assign (segid 3A4 and resid 71 and name CA) (segid 3A4 and resid 323 and name CB)	11.14	0.74	0.74
	assign (segid 3A4 and resid 71 and name CA) (segid 3A4 and resid 324 and name CA)	11.13	0.18	0.18
80	assign (segid 3A4 and resid 71 and name CA) (segid 3A4 and resid 324 and name CB)	10.67	0.41	0.40
	assign (segid 3A4 and resid 71 and name CA) (segid 3A4 and resid 325 and name CA)	12.45	0.48	0.49
	assign (segid 3A4 and resid 71 and name CA) (segid 3A4 and resid 325 and name CB)	13.90	0.47	0.47
	assign (segid 3A4 and resid 71 and name CA) (segid 3A4 and resid 326 and name CA)	11.28	0.71	0.71

	assign (segid 3A4 and resid 71 and name CA) (segid 3A4 and resid 326 and name CB)	10.34	0.92	0.92
	assign (segid 3A4 and resid 71 and name CA) (segid 3A4 and resid 327 and name CA)	14.56	0.87	0.87
	assign (segid 3A4 and resid 71 and name CA) (segid 3A4 and resid 327 and name CB)	14.67	0.99	0.98
	assign (segid 3A4 and resid 71 and name CA) (segid 3A4 and resid 328 and name CA)	17.77	0.80	0.79
5	assign (segid 3A4 and resid 71 and name CA) (segid 3A4 and resid 329 and name CB)	16.91	1.09	1.08
	assign (segid 3A4 and resid 71 and name CA) (segid 3A4 and resid 337 and name CB)	18.33	0.43	0.43
	assign (segid 3A4 and resid 71 and name CA) (segid 3A4 and resid 338 and name CA)	18.83	0.74	0.73
	assign (segid 3A4 and resid 71 and name CA) (segid 3A4 and resid 339 and name CA)	15.81	0.98	0.98
	assign (segid 3A4 and resid 71 and name CA) (segid 3A4 and resid 339 and name CB)	15.95	1.15	1.14
10	assign (segid 3A4 and resid 71 and name CA) (segid 3A4 and resid 340 and name CA)	14.46	1.25	1.25
	assign (segid 3A4 and resid 71 and name CA) (segid 3A4 and resid 341 and name CA)	16.13	0.76	0.76
	assign (segid 3A4 and resid 71 and name CA) (segid 3A4 and resid 341 and name CB)	17.06	0.59	0.59
	assign (segid 3A4 and resid 71 and name CA) (segid 3A4 and resid 342 and name CA)	15.08	0.57	0.57
	assign (segid 3A4 and resid 71 and name CA) (segid 3A4 and resid 343 and name CA)	15.71	0.12	0.11
15	assign (segid 3A4 and resid 71 and name CA) (segid 3A4 and resid 343 and name CB)	15.31	0.21	0.20
	assign (segid 3A4 and resid 71 and name CA) (segid 3A4 and resid 344 and name CA)	16.84	0.40	0.41
	assign (segid 3A4 and resid 71 and name CA) (segid 3A4 and resid 344 and name CB)	17.91	0.52	0.51
	assign (segid 3A4 and resid 71 and name CA) (segid 3A4 and resid 345 and name CA)	17.33	0.94	0.93
	assign (segid 3A4 and resid 71 and name CA) (segid 3A4 and resid 345 and name CB)	16.35	1.16	1.16
20	assign (segid 3A4 and resid 71 and name CA) (segid 3A4 and resid 385 and name CA)	15.83	1.26	1.26
	assign (segid 3A4 and resid 71 and name CA) (segid 3A4 and resid 386 and name CA)	15.04	1.48	1.47
	assign (segid 3A4 and resid 71 and name CA) (segid 3A4 and resid 387 and name CA)	12.71	1.34	1.34
	assign (segid 3A4 and resid 71 and name CA) (segid 3A4 and resid 388 and name CA)	10.11	1.48	1.48
	assign (segid 3A4 and resid 71 and name CA) (segid 3A4 and resid 388 and name CB)	9.07	1.74	1.74
25	assign (segid 3A4 and resid 71 and name CA) (segid 3A4 and resid 389 and name CA)	9.68	0.89	0.88
	assign (segid 3A4 and resid 71 and name CA) (segid 3A4 and resid 389 and name CB)	9.03	0.88	0.87
	assign (segid 3A4 and resid 71 and name CA) (segid 3A4 and resid 390 and name CA)	13.40	0.86	0.85
	assign (segid 3A4 and resid 71 and name CA) (segid 3A4 and resid 390 and name CB)	14.28	0.96	0.96
	assign (segid 3A4 and resid 71 and name CA) (segid 3A4 and resid 391 and name CA)	15.17	0.61	0.62
30	assign (segid 3A4 and resid 71 and name CA) (segid 3A4 and resid 391 and name CB)	16.48	0.66	0.66
	assign (segid 3A4 and resid 71 and name CA) (segid 3A4 and resid 392 and name CA)	15.54	0.38	0.39
	assign (segid 3A4 and resid 71 and name CA) (segid 3A4 and resid 393 and name CA)	14.78	0.32	0.32
	assign (segid 3A4 and resid 71 and name CA) (segid 3A4 and resid 393 and name CB)	18.80	0.44	0.44
	assign (segid 3A4 and resid 71 and name CA) (segid 3A4 and resid 71 and name C)	1.52	0.01	0.00
35	assign (segid 3A4 and resid 71 and name CA) (segid 3A4 and resid 71 and name CB)	1.54	0.01	0.01
	assign (segid 3A4 and resid 71 and name CA) (segid 3A4 and resid 71 and name CG)	2.68	0.20	0.20
	assign (segid 3A4 and resid 71 and name CA) (segid 3A4 and resid 71 and name O)	2.39	0.02	0.02
	assign (segid 3A4 and resid 71 and name CA) (segid 3A4 and resid 72 and name C)	4.36	0.06	0.06
	assign (segid 3A4 and resid 71 and name CA) (segid 3A4 and resid 72 and name CA)	3.81	0.01	0.02
40	assign (segid 3A4 and resid 71 and name CA) (segid 3A4 and resid 72 and name N)	2.44	0.02	0.02
	assign (segid 3A4 and resid 71 and name CA) (segid 3A4 and resid 72 and name O)	4.55	0.51	0.51
	assign (segid 3A4 and resid 71 and name CA) (segid 3A4 and resid 73 and name CA)	6.53	0.92	0.92
	assign (segid 3A4 and resid 71 and name CA) (segid 3A4 and resid 73 and name CB)	7.66	1.17	1.17
	assign (segid 3A4 and resid 71 and name CA) (segid 3A4 and resid 73 and name N)	5.62	0.87	0.87
45	assign (segid 3A4 and resid 71 and name CA) (segid 3A4 and resid 74 and name CA)	6.56	0.97	0.97
	assign (segid 3A4 and resid 71 and name CA) (segid 3A4 and resid 74 and name CB)	6.37	1.12	1.13
	assign (segid 3A4 and resid 71 and name CA) (segid 3A4 and resid 75 and name CA)	5.55	0.52	0.53
	assign (segid 3A4 and resid 71 and name CA) (segid 3A4 and resid 75 and name CB)	4.53	0.40	0.41
	assign (segid 3A4 and resid 71 and name CA) (segid 3A4 and resid 75 and name CG)	5.34	0.33	0.34
50	assign (segid 3A4 and resid 71 and name CA) (segid 3A4 and resid 75 and name N)	5.30	0.72	0.71
	assign (segid 3A4 and resid 71 and name CA) (segid 3A4 and resid 76 and name CA)	8.35	0.45	0.45
	assign (segid 3A4 and resid 71 and name CA) (segid 3A4 and resid 76 and name CB)	8.64	0.47	0.48
	assign (segid 3A4 and resid 71 and name CA) (segid 3A4 and resid 77 and name CA)	10.63	0.66	0.67
	assign (segid 3A4 and resid 71 and name CA) (segid 3A4 and resid 77 and name CB)	10.73	0.75	0.76
55	assign (segid 3A4 and resid 71 and name CA) (segid 3A4 and resid 78 and name CA)	10.70	0.58	0.59
	assign (segid 3A4 and resid 71 and name CA) (segid 3A4 and resid 78 and name CB)	9.95	0.61	0.60
	assign (segid 3A4 and resid 71 and name CA) (segid 3A4 and resid 79 and name CA)	11.01	0.33	0.32
	assign (segid 3A4 and resid 71 and name CA) (segid 3A4 and resid 79 and name CB)	10.14	0.29	0.30
	assign (segid 3A4 and resid 71 and name CA) (segid 3A4 and resid 80 and name CA)	13.65	0.47	0.47
60	assign (segid 3A4 and resid 71 and name CA) (segid 3A4 and resid 81 and name CA)	15.60	0.50	0.49
	assign (segid 3A4 and resid 71 and name CA) (segid 3A4 and resid 81 and name CB)	15.32	0.56	0.55
	assign (segid 3A4 and resid 71 and name CA) (segid 3A4 and resid 82 and name CA)	16.06	0.52	0.52
	assign (segid 3A4 and resid 71 and name CA) (segid 3A4 and resid 82 and name CB)	15.30	0.77	0.78
	assign (segid 3A4 and resid 71 and name CA) (segid 3A4 and resid 83 and name CA)	16.63	0.29	0.28
65	assign (segid 3A4 and resid 71 and name CA) (segid 3A4 and resid 83 and name CB)	15.97	0.43	0.42
	assign (segid 3A4 and resid 71 and name CB) (segid 3A4 and resid 243 and name CA)	15.38	1.39	1.40
	assign (segid 3A4 and resid 71 and name CB) (segid 3A4 and resid 243 and name CB)	14.77	1.41	1.40
	assign (segid 3A4 and resid 71 and name CB) (segid 3A4 and resid 246 and name CA)	16.16	1.14	1.14
	assign (segid 3A4 and resid 71 and name CB) (segid 3A4 and resid 246 and name CB)	14.93	1.21	1.21
70	assign (segid 3A4 and resid 71 and name CB) (segid 3A4 and resid 247 and name CA)	15.91	0.77	0.77
	assign (segid 3A4 and resid 71 and name CB) (segid 3A4 and resid 247 and name CB)	15.93	0.74	0.73
	assign (segid 3A4 and resid 71 and name CB) (segid 3A4 and resid 250 and name CA)	16.77	0.67	0.67
	assign (segid 3A4 and resid 71 and name CB) (segid 3A4 and resid 250 and name CB)	15.37	0.66	0.65
	assign (segid 3A4 and resid 71 and name CB) (segid 3A4 and resid 251 and name CA)	19.01	0.44	0.44
75	assign (segid 3A4 and resid 71 and name CB) (segid 3A4 and resid 322 and name CA)	13.09	0.65	0.64
	assign (segid 3A4 and resid 71 and name CB) (segid 3A4 and resid 323 and name CA)	10.87	0.81	0.82
	assign (segid 3A4 and resid 71 and name CB) (segid 3A4 and resid 323 and name CB)	11.11	1.23	1.22
	assign (segid 3A4 and resid 71 and name CB) (segid 3A4 and resid 324 and name CA)	10.65	0.38	0.37
	assign (segid 3A4 and resid 71 and name CB) (segid 3A4 and resid 324 and name CB)	10.12	0.28	0.28
80	assign (segid 3A4 and resid 71 and name CB) (segid 3A4 and resid 325 and name CA)	11.74	0.60	0.59
	assign (segid 3A4 and resid 71 and name CB) (segid 3A4 and resid 325 and name CB)	13.17	0.56	0.56
	assign (segid 3A4 and resid 71 and name CB) (segid 3A4 and resid 326 and name CA)	10.31	0.66	0.66
	assign (segid 3A4 and resid 71 and name CB) (segid 3A4 and resid 326 and name CB)	9.38	1.02	1.02

	assign (segid 3A4 and resid 71 and name CB) (segid 3A4 and resid 327 and name CA)	13.52	0.81	0.80
	assign (segid 3A4 and resid 71 and name CB) (segid 3A4 and resid 327 and name CB)	13.63	1.02	1.02
	assign (segid 3A4 and resid 71 and name CB) (segid 3A4 and resid 328 and name CA)	16.80	0.76	0.76
	assign (segid 3A4 and resid 71 and name CB) (segid 3A4 and resid 328 and name CB)	18.09	0.70	0.69
5	assign (segid 3A4 and resid 71 and name CB) (segid 3A4 and resid 329 and name CB)	16.21	1.40	1.39
	assign (segid 3A4 and resid 71 and name CB) (segid 3A4 and resid 337 and name CA)	18.66	0.57	0.57
	assign (segid 3A4 and resid 71 and name CB) (segid 3A4 and resid 337 and name CB)	17.67	0.69	0.68
	assign (segid 3A4 and resid 71 and name CB) (segid 3A4 and resid 338 and name CA)	17.89	0.40	0.40
	assign (segid 3A4 and resid 71 and name CB) (segid 3A4 and resid 338 and name CB)	18.78	0.42	0.43
10	assign (segid 3A4 and resid 71 and name CB) (segid 3A4 and resid 339 and name CA)	14.78	0.60	0.59
	assign (segid 3A4 and resid 71 and name CB) (segid 3A4 and resid 339 and name CB)	14.83	0.78	0.78
	assign (segid 3A4 and resid 71 and name CB) (segid 3A4 and resid 340 and name CA)	13.52	0.85	0.86
	assign (segid 3A4 and resid 71 and name CB) (segid 3A4 and resid 341 and name CA)	15.41	0.36	0.36
	assign (segid 3A4 and resid 71 and name CB) (segid 3A4 and resid 341 and name CB)	16.35	0.19	0.19
15	assign (segid 3A4 and resid 71 and name CB) (segid 3A4 and resid 342 and name CA)	14.65	0.33	0.33
	assign (segid 3A4 and resid 71 and name CB) (segid 3A4 and resid 343 and name CA)	15.52	0.44	0.43
	assign (segid 3A4 and resid 71 and name CB) (segid 3A4 and resid 343 and name CB)	15.10	0.57	0.58
	assign (segid 3A4 and resid 71 and name CB) (segid 3A4 and resid 344 and name CA)	16.94	0.66	0.67
	assign (segid 3A4 and resid 71 and name CB) (segid 3A4 and resid 344 and name CB)	18.00	0.58	0.58
20	assign (segid 3A4 and resid 71 and name CB) (segid 3A4 and resid 387 and name CA)	13.57	1.58	1.59
	assign (segid 3A4 and resid 71 and name CB) (segid 3A4 and resid 388 and name CA)	11.18	1.62	1.62
	assign (segid 3A4 and resid 71 and name CB) (segid 3A4 and resid 388 and name CB)	10.09	1.87	1.86
	assign (segid 3A4 and resid 71 and name CB) (segid 3A4 and resid 389 and name CA)	10.90	0.99	1.00
	assign (segid 3A4 and resid 71 and name CB) (segid 3A4 and resid 389 and name CB)	10.18	1.00	1.00
25	assign (segid 3A4 and resid 71 and name CB) (segid 3A4 and resid 390 and name CA)	14.62	0.98	0.97
	assign (segid 3A4 and resid 71 and name CB) (segid 3A4 and resid 390 and name CB)	15.48	1.09	1.09
	assign (segid 3A4 and resid 71 and name CB) (segid 3A4 and resid 391 and name CA)	16.50	0.67	0.68
	assign (segid 3A4 and resid 71 and name CB) (segid 3A4 and resid 391 and name CB)	17.78	0.72	0.72
	assign (segid 3A4 and resid 71 and name CB) (segid 3A4 and resid 392 and name CA)	16.98	0.37	0.38
30	assign (segid 3A4 and resid 71 and name CB) (segid 3A4 and resid 392 and name CB)	16.24	0.29	0.29
	assign (segid 3A4 and resid 71 and name CB) (segid 3A4 and resid 71 and name CG)	1.67	0.27	0.27
	assign (segid 3A4 and resid 71 and name CB) (segid 3A4 and resid 72 and name C)	4.63	0.10	0.10
	assign (segid 3A4 and resid 71 and name CB) (segid 3A4 and resid 72 and name CA)	4.48	0.06	0.06
	assign (segid 3A4 and resid 71 and name CB) (segid 3A4 and resid 72 and name N)	3.19	0.07	0.07
35	assign (segid 3A4 and resid 71 and name CB) (segid 3A4 and resid 72 and name O)	4.56	0.76	0.76
	assign (segid 3A4 and resid 71 and name CB) (segid 3A4 and resid 73 and name CA)	6.85	0.94	0.94
	assign (segid 3A4 and resid 71 and name CB) (segid 3A4 and resid 73 and name CB)	7.78	1.34	1.34
	assign (segid 3A4 and resid 71 and name CB) (segid 3A4 and resid 73 and name N)	5.78	0.82	0.82
	assign (segid 3A4 and resid 71 and name CB) (segid 3A4 and resid 74 and name CA)	7.27	0.91	0.92
40	assign (segid 3A4 and resid 71 and name CB) (segid 3A4 and resid 74 and name CB)	6.97	1.08	1.08
	assign (segid 3A4 and resid 71 and name CB) (segid 3A4 and resid 75 and name CA)	6.86	0.40	0.39
	assign (segid 3A4 and resid 71 and name CB) (segid 3A4 and resid 75 and name CB)	5.92	0.26	0.27
	assign (segid 3A4 and resid 71 and name CB) (segid 3A4 and resid 75 and name CG)	6.79	0.27	0.27
	assign (segid 3A4 and resid 71 and name CB) (segid 3A4 and resid 75 and name N)	6.41	0.59	0.58
45	assign (segid 3A4 and resid 71 and name CB) (segid 3A4 and resid 76 and name CA)	9.51	0.35	0.34
	assign (segid 3A4 and resid 71 and name CB) (segid 3A4 and resid 76 and name CB)	9.64	0.39	0.40
	assign (segid 3A4 and resid 71 and name CB) (segid 3A4 and resid 77 and name CA)	11.69	0.64	0.63
	assign (segid 3A4 and resid 71 and name CB) (segid 3A4 and resid 77 and name CB)	11.66	0.77	0.78
	assign (segid 3A4 and resid 71 and name CB) (segid 3A4 and resid 78 and name CA)	11.95	0.55	0.55
50	assign (segid 3A4 and resid 71 and name CB) (segid 3A4 and resid 78 and name CB)	11.18	0.57	0.57
	assign (segid 3A4 and resid 71 and name CB) (segid 3A4 and resid 79 and name CA)	12.42	0.26	0.25
	assign (segid 3A4 and resid 71 and name CB) (segid 3A4 and resid 79 and name CB)	11.56	0.20	0.21
	assign (segid 3A4 and resid 71 and name CB) (segid 3A4 and resid 80 and name CA)	14.95	0.40	0.40
	assign (segid 3A4 and resid 71 and name CB) (segid 3A4 and resid 81 and name CA)	16.89	0.48	0.47
55	assign (segid 3A4 and resid 71 and name CB) (segid 3A4 and resid 81 and name CB)	16.56	0.55	0.56
	assign (segid 3A4 and resid 71 and name CB) (segid 3A4 and resid 82 and name CA)	17.46	0.55	0.55
	assign (segid 3A4 and resid 71 and name CB) (segid 3A4 and resid 82 and name CB)	16.72	0.81	0.82
	assign (segid 3A4 and resid 71 and name CB) (segid 3A4 and resid 83 and name CA)	18.06	0.23	0.23
	assign (segid 3A4 and resid 71 and name CB) (segid 3A4 and resid 83 and name CB)	17.38	0.38	0.38
60	assign (segid 3A4 and resid 71 and name CB) (segid 3A4 and resid 72 and name C)	6.22	0.27	0.27
	assign (segid 3A4 and resid 71 and name CG) (segid 3A4 and resid 72 and name CA)	5.96	0.18	0.18
	assign (segid 3A4 and resid 71 and name CG) (segid 3A4 and resid 72 and name N)	4.59	0.18	0.18
	assign (segid 3A4 and resid 71 and name N) (segid 3A4 and resid 71 and name C)	2.41	0.06	0.07
	assign (segid 3A4 and resid 71 and name N) (segid 3A4 and resid 71 and name CA)	1.46	0.01	0.01
65	assign (segid 3A4 and resid 71 and name N) (segid 3A4 and resid 71 and name CB)	2.46	0.03	0.02
	assign (segid 3A4 and resid 71 and name N) (segid 3A4 and resid 71 and name CG)	3.20	0.18	0.18
	assign (segid 3A4 and resid 71 and name N) (segid 3A4 and resid 71 and name O)	2.66	0.14	0.13
	assign (segid 3A4 and resid 71 and name N) (segid 3A4 and resid 72 and name C)	5.28	0.11	0.10
	assign (segid 3A4 and resid 71 and name N) (segid 3A4 and resid 72 and name CA)	4.80	0.06	0.07
70	assign (segid 3A4 and resid 71 and name N) (segid 3A4 and resid 72 and name N)	3.59	0.03	0.04
	assign (segid 3A4 and resid 71 and name N) (segid 3A4 and resid 72 and name O)	5.45	0.43	0.43
	assign (segid 3A4 and resid 71 and name N) (segid 3A4 and resid 73 and name N)	6.25	0.53	0.52
	assign (segid 3A4 and resid 71 and name N) (segid 3A4 and resid 74 and name C)	6.05	0.63	0.64
	assign (segid 3A4 and resid 71 and name N) (segid 3A4 and resid 75 and name C)	6.71	0.41	0.41
75	assign (segid 3A4 and resid 71 and name N) (segid 3A4 and resid 75 and name CA)	5.30	0.46	0.45
	assign (segid 3A4 and resid 71 and name N) (segid 3A4 and resid 75 and name CB)	4.47	0.33	0.34
	assign (segid 3A4 and resid 71 and name N) (segid 3A4 and resid 75 and name CG)	5.33	0.34	0.33
	assign (segid 3A4 and resid 71 and name N) (segid 3A4 and resid 75 and name N)	5.06	0.58	0.59
	assign (segid 3A4 and resid 71 and name O) (segid 3A4 and resid 71 and name CB)	3.26	0.08	0.08
80	assign (segid 3A4 and resid 71 and name O) (segid 3A4 and resid 71 and name CG)	1.79	0.22	0.23
	assign (segid 3A4 and resid 71 and name O) (segid 3A4 and resid 72 and name C)	2.94	0.11	0.11
	assign (segid 3A4 and resid 71 and name O) (segid 3A4 and resid 72 and name CA)	2.76	0.06	0.05
	assign (segid 3A4 and resid 71 and name O) (segid 3A4 and resid 72 and name N)	2.24	0.02	0.02

	assign (segid 3A4 and resid 71 and name O) (segid 3A4 and resid 72 and name O)	3.34	0.10	0.10
	assign (segid 3A4 and resid 71 and name O) (segid 3A4 and resid 73 and name C)	4.42	0.90	0.90
	assign (segid 3A4 and resid 71 and name O) (segid 3A4 and resid 73 and name CA)	4.61	0.84	0.84
	assign (segid 3A4 and resid 71 and name O) (segid 3A4 and resid 73 and name N)	3.90	0.76	0.77
5	assign (segid 3A4 and resid 71 and name O) (segid 3A4 and resid 73 and name O)	5.30	0.77	0.77
	assign (segid 3A4 and resid 71 and name O) (segid 3A4 and resid 74 and name C)	4.24	0.81	0.80
	assign (segid 3A4 and resid 71 and name O) (segid 3A4 and resid 74 and name CA)	4.29	1.07	1.07
	assign (segid 3A4 and resid 71 and name O) (segid 3A4 and resid 74 and name CB)	4.33	1.25	1.24
	assign (segid 3A4 and resid 71 and name O) (segid 3A4 and resid 74 and name N)	3.76	1.11	1.12
10	assign (segid 3A4 and resid 71 and name O) (segid 3A4 and resid 74 and name O)	5.36	0.70	0.70
	assign (segid 3A4 and resid 71 and name O) (segid 3A4 and resid 75 and name C)	5.16	0.27	0.27
	assign (segid 3A4 and resid 71 and name O) (segid 3A4 and resid 75 and name CA)	3.98	0.32	0.33
	assign (segid 3A4 and resid 71 and name O) (segid 3A4 and resid 75 and name CB)	3.48	0.05	0.05
	assign (segid 3A4 and resid 71 and name O) (segid 3A4 and resid 75 and name CG)	4.72	0.29	0.29
15	assign (segid 3A4 and resid 71 and name O) (segid 3A4 and resid 75 and name N)	3.30	0.67	0.67
	assign (segid 3A4 and resid 71 and name O) (segid 3A4 and resid 75 and name O)	6.23	0.26	0.26
	assign (segid 3A4 and resid 71 and name O) (segid 3A4 and resid 76 and name CA)	6.64	0.25	0.26
	assign (segid 3A4 and resid 71 and name O) (segid 3A4 and resid 76 and name CB)	6.94	0.31	0.30
	assign (segid 3A4 and resid 71 and name O) (segid 3A4 and resid 76 and name N)	5.30	0.29	0.29
20	assign (segid 3A4 and resid 72 and name C) (segid 3A4 and resid 72 and name O)	1.24	0.01	0.01
	assign (segid 3A4 and resid 72 and name C) (segid 3A4 and resid 73 and name C)	3.91	1.18	1.19
	assign (segid 3A4 and resid 72 and name C) (segid 3A4 and resid 73 and name CA)	3.21	1.31	1.32
	assign (segid 3A4 and resid 72 and name C) (segid 3A4 and resid 73 and name N)	2.14	1.45	1.44
	assign (segid 3A4 and resid 72 and name C) (segid 3A4 and resid 73 and name O)	4.83	0.96	0.97
25	assign (segid 3A4 and resid 72 and name C) (segid 3A4 and resid 74 and name C)	5.45	0.82	0.81
	assign (segid 3A4 and resid 72 and name C) (segid 3A4 and resid 74 and name N)	4.04	1.30	1.30
	assign (segid 3A4 and resid 72 and name C) (segid 3A4 and resid 75 and name C)	5.99	0.61	0.61
	assign (segid 3A4 and resid 72 and name C) (segid 3A4 and resid 75 and name CA)	5.44	0.50	0.51
	assign (segid 3A4 and resid 72 and name C) (segid 3A4 and resid 75 and name CB)	4.99	0.48	0.48
30	assign (segid 3A4 and resid 72 and name C) (segid 3A4 and resid 75 and name CG)	6.02	0.67	0.67
	assign (segid 3A4 and resid 72 and name C) (segid 3A4 and resid 75 and name N)	4.74	0.67	0.66
	assign (segid 3A4 and resid 72 and name C) (segid 3A4 and resid 75 and name O)	7.15	0.66	0.65
	assign (segid 3A4 and resid 72 and name C) (segid 3A4 and resid 76 and name CA)	6.43	0.66	0.66
	assign (segid 3A4 and resid 72 and name C) (segid 3A4 and resid 76 and name CB)	6.12	0.71	0.70
35	assign (segid 3A4 and resid 72 and name C) (segid 3A4 and resid 76 and name N)	5.50	0.63	0.62
	assign (segid 3A4 and resid 72 and name CA) (segid 3A4 and resid 243 and name CA)	15.52	1.26	1.25
	assign (segid 3A4 and resid 72 and name CA) (segid 3A4 and resid 243 and name CB)	14.61	1.28	1.27
	assign (segid 3A4 and resid 72 and name CA) (segid 3A4 and resid 244 and name CA)	17.78	1.07	1.09
	assign (segid 3A4 and resid 72 and name CA) (segid 3A4 and resid 246 and name CA)	16.90	1.07	1.07
40	assign (segid 3A4 and resid 72 and name CA) (segid 3A4 and resid 246 and name CB)	15.85	1.11	1.10
	assign (segid 3A4 and resid 72 and name CA) (segid 3A4 and resid 247 and name CA)	15.76	0.84	0.84
	assign (segid 3A4 and resid 72 and name CA) (segid 3A4 and resid 247 and name CB)	15.40	0.79	0.79
	assign (segid 3A4 and resid 72 and name CA) (segid 3A4 and resid 250 and name CA)	17.30	0.94	0.95
	assign (segid 3A4 and resid 72 and name CA) (segid 3A4 and resid 250 and name CB)	15.81	0.94	0.95
45	assign (segid 3A4 and resid 72 and name CA) (segid 3A4 and resid 251 and name CA)	18.79	0.77	0.77
	assign (segid 3A4 and resid 72 and name CA) (segid 3A4 and resid 251 and name CB)	18.98	0.68	0.67
	assign (segid 3A4 and resid 72 and name CA) (segid 3A4 and resid 322 and name CA)	15.47	0.97	0.98
	assign (segid 3A4 and resid 72 and name CA) (segid 3A4 and resid 323 and name CA)	13.31	0.75	0.75
	assign (segid 3A4 and resid 72 and name CA) (segid 3A4 and resid 323 and name CB)	13.23	0.51	0.50
50	assign (segid 3A4 and resid 72 and name CA) (segid 3A4 and resid 324 and name CA)	13.61	0.99	0.99
	assign (segid 3A4 and resid 72 and name CA) (segid 3A4 and resid 324 and name CB)	13.36	1.15	1.15
	assign (segid 3A4 and resid 72 and name CA) (segid 3A4 and resid 325 and name CA)	14.22	0.95	0.95
	assign (segid 3A4 and resid 72 and name CA) (segid 3A4 and resid 325 and name CB)	15.61	0.94	0.94
55	assign (segid 3A4 and resid 72 and name CA) (segid 3A4 and resid 326 and name CA)	12.59	1.16	1.16
	assign (segid 3A4 and resid 72 and name CA) (segid 3A4 and resid 326 and name CB)	11.36	1.11	1.11
	assign (segid 3A4 and resid 72 and name CA) (segid 3A4 and resid 327 and name CA)	15.53	1.05	1.06
	assign (segid 3A4 and resid 72 and name CA) (segid 3A4 and resid 327 and name CB)	15.29	1.01	1.01
	assign (segid 3A4 and resid 72 and name CA) (segid 3A4 and resid 328 and name CA)	18.79	0.99	0.98
60	assign (segid 3A4 and resid 72 and name CA) (segid 3A4 and resid 329 and name CB)	17.64	0.59	0.59
	assign (segid 3A4 and resid 72 and name CA) (segid 3A4 and resid 339 and name CA)	17.59	1.43	1.43
	assign (segid 3A4 and resid 72 and name CA) (segid 3A4 and resid 339 and name CB)	17.59	1.56	1.56
	assign (segid 3A4 and resid 72 and name CA) (segid 3A4 and resid 340 and name CA)	16.87	1.74	1.74
	assign (segid 3A4 and resid 72 and name CA) (segid 3A4 and resid 342 and name CA)	17.82	1.21	1.20
65	assign (segid 3A4 and resid 72 and name CA) (segid 3A4 and resid 343 and name CA)	18.05	0.82	0.82
	assign (segid 3A4 and resid 72 and name CA) (segid 3A4 and resid 343 and name CB)	17.40	0.74	0.74
	assign (segid 3A4 and resid 72 and name CA) (segid 3A4 and resid 345 and name CB)	18.02	0.64	0.63
	assign (segid 3A4 and resid 72 and name CA) (segid 3A4 and resid 385 and name CA)	16.43	1.10	1.10
	assign (segid 3A4 and resid 72 and name CA) (segid 3A4 and resid 386 and name CA)	14.95	1.25	1.25
	assign (segid 3A4 and resid 72 and name CA) (segid 3A4 and resid 387 and name CA)	12.02	0.95	0.95
70	assign (segid 3A4 and resid 72 and name CA) (segid 3A4 and resid 388 and name CA)	9.01	0.94	0.93
	assign (segid 3A4 and resid 72 and name CA) (segid 3A4 and resid 388 and name CB)	7.77	1.09	1.09
	assign (segid 3A4 and resid 72 and name CA) (segid 3A4 and resid 389 and name CA)	9.77	0.82	0.82
	assign (segid 3A4 and resid 72 and name CA) (segid 3A4 and resid 389 and name CB)	9.61	0.97	0.97
	assign (segid 3A4 and resid 72 and name CA) (segid 3A4 and resid 390 and name CA)	13.28	0.74	0.74
75	assign (segid 3A4 and resid 72 and name CA) (segid 3A4 and resid 390 and name CB)	13.84	0.73	0.72
	assign (segid 3A4 and resid 72 and name CA) (segid 3A4 and resid 391 and name CA)	15.40	0.69	0.69
	assign (segid 3A4 and resid 72 and name CA) (segid 3A4 and resid 391 and name CB)	16.84	0.71	0.71
	assign (segid 3A4 and resid 72 and name CA) (segid 3A4 and resid 392 and name CA)	15.26	0.62	0.61
	assign (segid 3A4 and resid 72 and name CA) (segid 3A4 and resid 392 and name CB)	14.53	0.66	0.66
80	assign (segid 3A4 and resid 72 and name CA) (segid 3A4 and resid 393 and name CA)	18.83	0.68	0.69
	assign (segid 3A4 and resid 72 and name CA) (segid 3A4 and resid 72 and name C)	1.54	0.01	0.01
	assign (segid 3A4 and resid 72 and name CA) (segid 3A4 and resid 72 and name O)	2.42	0.02	0.02
	assign (segid 3A4 and resid 72 and name CA) (segid 3A4 and resid 73 and name CA)	3.95	1.51	1.51

	assign (segid 3A4 and resid 72 and name CA) (segid 3A4 and resid 73 and name CB)	5.27	1.54	1.55
	assign (segid 3A4 and resid 72 and name CA) (segid 3A4 and resid 73 and name N)	3.27	1.46	1.47
	assign (segid 3A4 and resid 72 and name CA) (segid 3A4 and resid 74 and name C)	5.45	0.91	0.91
	assign (segid 3A4 and resid 72 and name CA) (segid 3A4 and resid 74 and name CA)	5.60	1.20	1.20
5	assign (segid 3A4 and resid 72 and name CA) (segid 3A4 and resid 74 and name CB)	6.27	1.27	1.27
	assign (segid 3A4 and resid 72 and name CA) (segid 3A4 and resid 75 and name C)	5.39	0.48	0.47
	assign (segid 3A4 and resid 72 and name CA) (segid 3A4 and resid 75 and name CA)	4.84	0.46	0.46
	assign (segid 3A4 and resid 72 and name CA) (segid 3A4 and resid 75 and name CB)	4.10	0.29	0.28
	assign (segid 3A4 and resid 72 and name CA) (segid 3A4 and resid 75 and name CG)	4.92	0.39	0.39
10	assign (segid 3A4 and resid 72 and name CA) (segid 3A4 and resid 75 and name N)	4.47	0.77	0.78
	assign (segid 3A4 and resid 72 and name CA) (segid 3A4 and resid 75 and name O)	6.54	0.42	0.41
	assign (segid 3A4 and resid 72 and name CA) (segid 3A4 and resid 76 and name CA)	5.90	0.57	0.56
	assign (segid 3A4 and resid 72 and name CA) (segid 3A4 and resid 76 and name CB)	5.71	0.70	0.69
	assign (segid 3A4 and resid 72 and name CA) (segid 3A4 and resid 76 and name N)	4.92	0.60	0.60
15	assign (segid 3A4 and resid 72 and name CA) (segid 3A4 and resid 77 and name CA)	8.53	0.84	0.85
	assign (segid 3A4 and resid 72 and name CA) (segid 3A4 and resid 77 and name CB)	8.72	0.98	0.99
	assign (segid 3A4 and resid 72 and name CA) (segid 3A4 and resid 78 and name CA)	9.78	0.56	0.55
	assign (segid 3A4 and resid 72 and name CA) (segid 3A4 and resid 78 and name CB)	9.53	0.53	0.53
	assign (segid 3A4 and resid 72 and name CA) (segid 3A4 and resid 79 and name CA)	9.82	0.37	0.36
20	assign (segid 3A4 and resid 72 and name CA) (segid 3A4 and resid 79 and name CB)	8.87	0.41	0.41
	assign (segid 3A4 and resid 72 and name CA) (segid 3A4 and resid 80 and name CA)	11.60	0.48	0.47
	assign (segid 3A4 and resid 72 and name CA) (segid 3A4 and resid 81 and name CA)	14.06	0.55	0.56
	assign (segid 3A4 and resid 72 and name CA) (segid 3A4 and resid 81 and name CB)	13.99	0.62	0.63
	assign (segid 3A4 and resid 72 and name CA) (segid 3A4 and resid 82 and name CA)	15.10	0.62	0.61
25	assign (segid 3A4 and resid 72 and name CA) (segid 3A4 and resid 82 and name CB)	14.65	0.90	0.89
	assign (segid 3A4 and resid 72 and name CA) (segid 3A4 and resid 83 and name CA)	15.20	0.40	0.40
	assign (segid 3A4 and resid 72 and name CA) (segid 3A4 and resid 83 and name CB)	14.30	0.40	0.40
	assign (segid 3A4 and resid 72 and name CA) (segid 3A4 and resid 84 and name CA)	18.07	0.49	0.48
	assign (segid 3A4 and resid 72 and name CA) (segid 3A4 and resid 84 and name CB)	18.20	0.70	0.70
30	assign (segid 3A4 and resid 72 and name CA) (segid 3A4 and resid 86 and name CB)	18.52	0.62	0.62
	assign (segid 3A4 and resid 72 and name N) (segid 3A4 and resid 72 and name C)	2.44	0.02	0.03
	assign (segid 3A4 and resid 72 and name N) (segid 3A4 and resid 72 and name O)	1.46	0.00	0.01
	assign (segid 3A4 and resid 72 and name N) (segid 3A4 and resid 72 and name N)	2.99	0.34	0.33
	assign (segid 3A4 and resid 72 and name N) (segid 3A4 and resid 73 and name N)	4.15	1.29	1.28
35	assign (segid 3A4 and resid 72 and name N) (segid 3A4 and resid 75 and name C)	5.86	0.50	0.50
	assign (segid 3A4 and resid 72 and name N) (segid 3A4 and resid 75 and name CA)	5.01	0.53	0.52
	assign (segid 3A4 and resid 72 and name N) (segid 3A4 and resid 75 and name CB)	4.01	0.33	0.34
	assign (segid 3A4 and resid 72 and name N) (segid 3A4 and resid 75 and name CG)	4.81	0.19	0.19
	assign (segid 3A4 and resid 72 and name N) (segid 3A4 and resid 75 and name N)	4.73	0.82	0.82
40	assign (segid 3A4 and resid 72 and name N) (segid 3A4 and resid 76 and name N)	5.67	0.58	0.58
	assign (segid 3A4 and resid 72 and name O) (segid 3A4 and resid 73 and name C)	4.47	0.89	0.88
	assign (segid 3A4 and resid 72 and name O) (segid 3A4 and resid 73 and name CA)	3.90	0.85	0.84
	assign (segid 3A4 and resid 72 and name O) (segid 3A4 and resid 73 and name CB)	4.95	0.95	0.95
45	assign (segid 3A4 and resid 72 and name O) (segid 3A4 and resid 73 and name N)	2.81	1.03	1.03
	assign (segid 3A4 and resid 72 and name O) (segid 3A4 and resid 73 and name O)	5.34	0.85	0.86
	assign (segid 3A4 and resid 72 and name O) (segid 3A4 and resid 74 and name C)	5.82	0.88	0.87
	assign (segid 3A4 and resid 72 and name O) (segid 3A4 and resid 74 and name CA)	5.54	0.94	0.93
	assign (segid 3A4 and resid 72 and name O) (segid 3A4 and resid 74 and name N)	4.48	1.01	1.00
50	assign (segid 3A4 and resid 72 and name O) (segid 3A4 and resid 75 and name C)	6.87	0.92	0.93
	assign (segid 3A4 and resid 72 and name O) (segid 3A4 and resid 75 and name CA)	5.85	0.90	0.90
	assign (segid 3A4 and resid 72 and name O) (segid 3A4 and resid 75 and name CB)	5.42	0.82	0.82
	assign (segid 3A4 and resid 72 and name O) (segid 3A4 and resid 75 and name CG)	6.43	1.02	1.02
	assign (segid 3A4 and resid 72 and name O) (segid 3A4 and resid 75 and name N)	5.14	0.81	0.81
55	assign (segid 3A4 and resid 72 and name O) (segid 3A4 and resid 76 and name N)	5.95	1.26	1.25
	assign (segid 3A4 and resid 73 and name C) (segid 3A4 and resid 73 and name CB)	2.52	0.01	0.01
	assign (segid 3A4 and resid 73 and name C) (segid 3A4 and resid 73 and name O)	1.24	0.02	0.01
	assign (segid 3A4 and resid 73 and name C) (segid 3A4 and resid 74 and name C)	3.09	0.12	0.11
60	assign (segid 3A4 and resid 73 and name C) (segid 3A4 and resid 74 and name CB)	2.44	0.01	0.01
	assign (segid 3A4 and resid 73 and name C) (segid 3A4 and resid 74 and name N)	3.70	0.05	0.04
	assign (segid 3A4 and resid 73 and name C) (segid 3A4 and resid 74 and name O)	1.33	0.01	0.01
	assign (segid 3A4 and resid 73 and name C) (segid 3A4 and resid 75 and name C)	3.95	0.19	0.19
	assign (segid 3A4 and resid 73 and name C) (segid 3A4 and resid 75 and name CA)	4.71	0.22	0.21
65	assign (segid 3A4 and resid 73 and name C) (segid 3A4 and resid 75 and name CB)	4.53	0.16	0.15
	assign (segid 3A4 and resid 73 and name C) (segid 3A4 and resid 75 and name CG)	5.16	0.18	0.18
	assign (segid 3A4 and resid 73 and name C) (segid 3A4 and resid 75 and name N)	6.46	0.20	0.21
	assign (segid 3A4 and resid 73 and name C) (segid 3A4 and resid 75 and name O)	3.31	0.11	0.12
	assign (segid 3A4 and resid 73 and name C) (segid 3A4 and resid 76 and name C)	5.68	0.11	0.12
70	assign (segid 3A4 and resid 73 and name C) (segid 3A4 and resid 76 and name CA)	5.44	0.37	0.38
	assign (segid 3A4 and resid 73 and name C) (segid 3A4 and resid 76 and name CB)	5.00	0.44	0.45
	assign (segid 3A4 and resid 73 and name C) (segid 3A4 and resid 76 and name N)	4.83	0.55	0.55
	assign (segid 3A4 and resid 73 and name C) (segid 3A4 and resid 76 and name O)	4.20	0.44	0.44
	assign (segid 3A4 and resid 73 and name C) (segid 3A4 and resid 77 and name C)	6.64	0.36	0.37
75	assign (segid 3A4 and resid 73 and name C) (segid 3A4 and resid 77 and name CA)	6.64	0.46	0.46
	assign (segid 3A4 and resid 73 and name C) (segid 3A4 and resid 77 and name CB)	5.64	0.50	0.50
	assign (segid 3A4 and resid 73 and name C) (segid 3A4 and resid 77 and name N)	5.20	0.66	0.66
	assign (segid 3A4 and resid 73 and name C) (segid 3A4 and resid 78 and name N)	4.75	0.43	0.42
	assign (segid 3A4 and resid 73 and name C) (segid 3A4 and resid 224 and name CA)	6.40	0.40	0.40
80	assign (segid 3A4 and resid 73 and name CA) (segid 3A4 and resid 224 and name CB)	18.24	1.07	1.07
	assign (segid 3A4 and resid 73 and name CA) (segid 3A4 and resid 240 and name CA)	17.97	1.08	1.09
	assign (segid 3A4 and resid 73 and name CA) (segid 3A4 and resid 240 and name CB)	15.87	2.03	2.02
	assign (segid 3A4 and resid 73 and name CA) (segid 3A4 and resid 243 and name CA)	15.40	2.21	2.21
	assign (segid 3A4 and resid 73 and name CA) (segid 3A4 and resid 243 and name CB)	14.34	1.79	1.79

	assign (segid 3A4 and resid 73 and name CA) (segid 3A4 and resid 243 and name CB)	13.19	1.86	1.86
	assign (segid 3A4 and resid 73 and name CA) (segid 3A4 and resid 244 and name CA)	16.73	1.54	1.55
	assign (segid 3A4 and resid 73 and name CA) (segid 3A4 and resid 244 and name CB)	17.69	1.55	1.56
	assign (segid 3A4 and resid 73 and name CA) (segid 3A4 and resid 246 and name CA)	16.85	1.42	1.41
5	assign (segid 3A4 and resid 73 and name CA) (segid 3A4 and resid 246 and name CB)	15.74	1.50	1.50
	assign (segid 3A4 and resid 73 and name CA) (segid 3A4 and resid 247 and name CA)	15.88	0.98	0.99
	assign (segid 3A4 and resid 73 and name CA) (segid 3A4 and resid 247 and name CB)	15.29	0.93	0.92
	assign (segid 3A4 and resid 73 and name CA) (segid 3A4 and resid 250 and name CA)	18.43	0.87	0.87
	assign (segid 3A4 and resid 73 and name CA) (segid 3A4 and resid 250 and name CB)	16.94	0.86	0.87
10	assign (segid 3A4 and resid 73 and name CA) (segid 3A4 and resid 323 and name CA)	17.08	0.84	0.83
	assign (segid 3A4 and resid 73 and name CA) (segid 3A4 and resid 324 and name CA)	17.10	0.91	0.92
	assign (segid 3A4 and resid 73 and name CA) (segid 3A4 and resid 324 and name CB)	16.68	0.85	0.86
	assign (segid 3A4 and resid 73 and name CA) (segid 3A4 and resid 326 and name CA)	15.50	1.40	1.41
	assign (segid 3A4 and resid 73 and name CA) (segid 3A4 and resid 326 and name CB)	14.25	1.56	1.56
15	assign (segid 3A4 and resid 73 and name CA) (segid 3A4 and resid 387 and name CA)	15.29	1.62	1.62
	assign (segid 3A4 and resid 73 and name CA) (segid 3A4 and resid 388 and name CA)	11.98	1.61	1.61
	assign (segid 3A4 and resid 73 and name CA) (segid 3A4 and resid 388 and name CB)	10.76	1.78	1.77
	assign (segid 3A4 and resid 73 and name CA) (segid 3A4 and resid 389 and name CA)	12.96	0.84	0.83
	assign (segid 3A4 and resid 73 and name CA) (segid 3A4 and resid 389 and name CB)	13.03	0.71	0.70
20	assign (segid 3A4 and resid 73 and name CA) (segid 3A4 and resid 390 and name CA)	16.23	0.96	0.97
	assign (segid 3A4 and resid 73 and name CA) (segid 3A4 and resid 390 and name CB)	16.71	1.20	1.20
	assign (segid 3A4 and resid 73 and name CA) (segid 3A4 and resid 391 and name CA)	17.94	0.55	0.56
	assign (segid 3A4 and resid 73 and name CA) (segid 3A4 and resid 392 and name CA)	17.08	0.32	0.33
	assign (segid 3A4 and resid 73 and name CA) (segid 3A4 and resid 392 and name CB)	16.15	0.21	0.21
25	assign (segid 3A4 and resid 73 and name CA) (segid 3A4 and resid 73 and name C)	1.53	0.01	0.00
	assign (segid 3A4 and resid 73 and name CA) (segid 3A4 and resid 73 and name CB)	1.53	0.02	0.01
	assign (segid 3A4 and resid 73 and name CA) (segid 3A4 and resid 73 and name O)	2.40	0.01	0.00
	assign (segid 3A4 and resid 73 and name CA) (segid 3A4 and resid 74 and name C)	4.47	0.07	0.06
	assign (segid 3A4 and resid 73 and name CA) (segid 3A4 and resid 74 and name CA)	3.82	0.01	0.02
30	assign (segid 3A4 and resid 73 and name CA) (segid 3A4 and resid 74 and name CB)	4.86	0.05	0.05
	assign (segid 3A4 and resid 73 and name CA) (segid 3A4 and resid 74 and name N)	2.44	0.01	0.02
	assign (segid 3A4 and resid 73 and name CA) (segid 3A4 and resid 74 and name O)	5.40	0.16	0.16
	assign (segid 3A4 and resid 73 and name CA) (segid 3A4 and resid 75 and name C)	5.70	0.17	0.17
	assign (segid 3A4 and resid 73 and name CA) (segid 3A4 and resid 75 and name CA)	5.50	0.08	0.09
35	assign (segid 3A4 and resid 73 and name CA) (segid 3A4 and resid 75 and name CB)	5.78	0.13	0.12
	assign (segid 3A4 and resid 73 and name CA) (segid 3A4 and resid 75 and name CG)	7.03	0.17	0.17
	assign (segid 3A4 and resid 73 and name CA) (segid 3A4 and resid 75 and name N)	4.40	0.05	0.05
	assign (segid 3A4 and resid 73 and name CA) (segid 3A4 and resid 75 and name O)	6.77	0.12	0.12
	assign (segid 3A4 and resid 73 and name CA) (segid 3A4 and resid 76 and name C)	6.35	0.37	0.37
40	assign (segid 3A4 and resid 73 and name CA) (segid 3A4 and resid 76 and name CA)	5.69	0.43	0.43
	assign (segid 3A4 and resid 73 and name CA) (segid 3A4 and resid 76 and name CB)	5.16	0.56	0.56
	assign (segid 3A4 and resid 73 and name CA) (segid 3A4 and resid 76 and name N)	5.00	0.37	0.37
	assign (segid 3A4 and resid 73 and name CA) (segid 3A4 and resid 77 and name CA)	6.83	0.52	0.51
	assign (segid 3A4 and resid 73 and name CA) (segid 3A4 and resid 77 and name CB)	6.45	0.68	0.67
45	assign (segid 3A4 and resid 73 and name CA) (segid 3A4 and resid 77 and name N)	5.84	0.44	0.44
	assign (segid 3A4 and resid 73 and name CA) (segid 3A4 and resid 78 and name CA)	9.03	0.33	0.34
	assign (segid 3A4 and resid 73 and name CA) (segid 3A4 and resid 78 and name CB)	9.03	0.35	0.34
	assign (segid 3A4 and resid 73 and name CA) (segid 3A4 and resid 79 and name CA)	10.21	0.19	0.18
	assign (segid 3A4 and resid 73 and name CA) (segid 3A4 and resid 79 and name CB)	9.68	0.20	0.21
50	assign (segid 3A4 and resid 73 and name CA) (segid 3A4 and resid 80 and name CA)	11.13	0.45	0.45
	assign (segid 3A4 and resid 73 and name CA) (segid 3A4 and resid 81 and name CA)	13.14	0.46	0.47
	assign (segid 3A4 and resid 73 and name CA) (segid 3A4 and resid 81 and name CB)	12.85	0.55	0.55
	assign (segid 3A4 and resid 73 and name CA) (segid 3A4 and resid 82 and name CA)	15.01	0.40	0.41
	assign (segid 3A4 and resid 73 and name CA) (segid 3A4 and resid 82 and name CB)	14.79	0.64	0.64
55	assign (segid 3A4 and resid 73 and name CA) (segid 3A4 and resid 83 and name CA)	15.60	0.42	0.42
	assign (segid 3A4 and resid 73 and name CA) (segid 3A4 and resid 83 and name CB)	14.74	0.60	0.59
	assign (segid 3A4 and resid 73 and name CA) (segid 3A4 and resid 84 and name CA)	17.96	0.43	0.43
	assign (segid 3A4 and resid 73 and name CA) (segid 3A4 and resid 84 and name CB)	17.83	0.58	0.58
60	assign (segid 3A4 and resid 73 and name CB) (segid 3A4 and resid 240 and name CA)	16.00	2.28	2.28
	assign (segid 3A4 and resid 73 and name CB) (segid 3A4 and resid 240 and name CB)	15.49	2.50	2.51
	assign (segid 3A4 and resid 73 and name CB) (segid 3A4 and resid 243 and name CA)	14.87	2.06	2.05
	assign (segid 3A4 and resid 73 and name CB) (segid 3A4 and resid 243 and name CB)	13.67	2.09	2.09
	assign (segid 3A4 and resid 73 and name CB) (segid 3A4 and resid 244 and name CA)	17.32	1.75	1.75
65	assign (segid 3A4 and resid 73 and name CB) (segid 3A4 and resid 246 and name CB)	16.52	1.81	1.81
	assign (segid 3A4 and resid 73 and name CB) (segid 3A4 and resid 247 and name CA)	16.81	1.18	1.18
	assign (segid 3A4 and resid 73 and name CB) (segid 3A4 and resid 247 and name CB)	16.18	1.09	1.08
	assign (segid 3A4 and resid 73 and name CB) (segid 3A4 and resid 250 and name CB)	18.06	1.10	1.10
	assign (segid 3A4 and resid 73 and name CB) (segid 3A4 and resid 324 and name CB)	17.64	1.13	1.14
	assign (segid 3A4 and resid 73 and name CB) (segid 3A4 and resid 326 and name CA)	16.20	1.59	1.58
70	assign (segid 3A4 and resid 73 and name CB) (segid 3A4 and resid 326 and name CB)	14.95	1.72	1.72
	assign (segid 3A4 and resid 73 and name CB) (segid 3A4 and resid 387 and name CA)	16.50	1.71	1.71
	assign (segid 3A4 and resid 73 and name CB) (segid 3A4 and resid 388 and name CA)	13.25	1.69	1.68
	assign (segid 3A4 and resid 73 and name CB) (segid 3A4 and resid 388 and name CB)	12.03	1.84	1.83
	assign (segid 3A4 and resid 73 and name CB) (segid 3A4 and resid 389 and name CA)	14.34	0.82	0.81
75	assign (segid 3A4 and resid 73 and name CB) (segid 3A4 and resid 389 and name CB)	14.42	0.65	0.65
	assign (segid 3A4 and resid 73 and name CB) (segid 3A4 and resid 390 and name CA)	17.55	0.99	1.00
	assign (segid 3A4 and resid 73 and name CB) (segid 3A4 and resid 392 and name CA)	18.32	0.36	0.36
	assign (segid 3A4 and resid 73 and name CB) (segid 3A4 and resid 392 and name CB)	17.37	0.22	0.22
80	assign (segid 3A4 and resid 73 and name CB) (segid 3A4 and resid 74 and name C)	5.52	0.03	0.03
	assign (segid 3A4 and resid 73 and name CB) (segid 3A4 and resid 74 and name CA)	4.63	0.09	0.09
	assign (segid 3A4 and resid 73 and name CB) (segid 3A4 and resid 74 and name CB)	5.56	0.22	0.22
	assign (segid 3A4 and resid 73 and name CB) (segid 3A4 and resid 74 and name N)	3.34	0.11	0.11
	assign (segid 3A4 and resid 73 and name CB) (segid 3A4 and resid 74 and name O)	6.36	0.16	0.16

	assign (segid 3A4 and resid 73 and name CB)	(segid 3A4 and resid 75 and name C)	6.97	0.19	0.19
	assign (segid 3A4 and resid 73 and name CB)	(segid 3A4 and resid 75 and name CA)	6.84	0.04	0.04
	assign (segid 3A4 and resid 73 and name CB)	(segid 3A4 and resid 75 and name CB)	7.19	0.11	0.11
	assign (segid 3A4 and resid 73 and name CB)	(segid 3A4 and resid 75 and name N)	5.67	0.07	0.06
5	assign (segid 3A4 and resid 73 and name CB)	(segid 3A4 and resid 76 and name CA)	6.76	0.57	0.57
	assign (segid 3A4 and resid 73 and name CB)	(segid 3A4 and resid 76 and name CB)	6.08	0.75	0.75
	assign (segid 3A4 and resid 73 and name CB)	(segid 3A4 and resid 76 and name N)	6.23	0.43	0.43
	assign (segid 3A4 and resid 73 and name CB)	(segid 3A4 and resid 77 and name CA)	7.44	0.65	0.65
	assign (segid 3A4 and resid 73 and name CB)	(segid 3A4 and resid 77 and name CB)	6.86	0.75	0.76
10	assign (segid 3A4 and resid 73 and name CB)	(segid 3A4 and resid 77 and name N)	6.64	0.57	0.57
	assign (segid 3A4 and resid 73 and name CB)	(segid 3A4 and resid 78 and name CA)	9.92	0.40	0.39
	assign (segid 3A4 and resid 73 and name CB)	(segid 3A4 and resid 78 and name CB)	9.96	0.38	0.39
	assign (segid 3A4 and resid 73 and name CB)	(segid 3A4 and resid 79 and name CA)	11.29	0.25	0.26
	assign (segid 3A4 and resid 73 and name CB)	(segid 3A4 and resid 79 and name CB)	10.86	0.26	0.26
15	assign (segid 3A4 and resid 73 and name CB)	(segid 3A4 and resid 80 and name CA)	11.91	0.64	0.64
	assign (segid 3A4 and resid 73 and name CB)	(segid 3A4 and resid 81 and name CA)	13.83	0.58	0.57
	assign (segid 3A4 and resid 73 and name CB)	(segid 3A4 and resid 81 and name CB)	13.50	0.62	0.63
	assign (segid 3A4 and resid 73 and name CB)	(segid 3A4 and resid 82 and name CA)	15.91	0.40	0.40
	assign (segid 3A4 and resid 73 and name CB)	(segid 3A4 and resid 82 and name CB)	15.76	0.60	0.59
20	assign (segid 3A4 and resid 73 and name CB)	(segid 3A4 and resid 83 and name CA)	16.54	0.57	0.58
	assign (segid 3A4 and resid 73 and name CB)	(segid 3A4 and resid 83 and name CB)	15.67	0.77	0.78
	assign (segid 3A4 and resid 73 and name CB)	(segid 3A4 and resid 84 and name CA)	18.73	0.57	0.57
	assign (segid 3A4 and resid 73 and name CB)	(segid 3A4 and resid 84 and name CB)	18.52	0.66	0.66
	assign (segid 3A4 and resid 73 and name N)	(segid 3A4 and resid 73 and name C)	2.50	0.03	0.03
25	assign (segid 3A4 and resid 73 and name N)	(segid 3A4 and resid 73 and name CB)	1.46	0.01	0.01
	assign (segid 3A4 and resid 73 and name N)	(segid 3A4 and resid 73 and name O)	3.60	0.06	0.06
	assign (segid 3A4 and resid 73 and name N)	(segid 3A4 and resid 74 and name C)	4.89	0.12	0.12
	assign (segid 3A4 and resid 73 and name N)	(segid 3A4 and resid 74 and name CA)	4.22	0.05	0.06
	assign (segid 3A4 and resid 73 and name N)	(segid 3A4 and resid 74 and name CB)	4.93	0.14	0.15
30	assign (segid 3A4 and resid 73 and name N)	(segid 3A4 and resid 74 and name N)	2.80	0.05	0.05
	assign (segid 3A4 and resid 73 and name N)	(segid 3A4 and resid 75 and name C)	5.98	0.10	0.10
	assign (segid 3A4 and resid 73 and name N)	(segid 3A4 and resid 75 and name CA)	6.18	0.28	0.27
	assign (segid 3A4 and resid 73 and name N)	(segid 3A4 and resid 75 and name CB)	5.70	0.26	0.25
35	assign (segid 3A4 and resid 73 and name N)	(segid 3A4 and resid 75 and name CG)	5.70	0.28	0.28
	assign (segid 3A4 and resid 73 and name N)	(segid 3A4 and resid 75 and name N)	6.99	0.28	0.29
	assign (segid 3A4 and resid 73 and name N)	(segid 3A4 and resid 75 and name O)	4.58	0.21	0.22
	assign (segid 3A4 and resid 73 and name N)	(segid 3A4 and resid 76 and name CA)	7.33	0.33	0.33
	assign (segid 3A4 and resid 73 and name N)	(segid 3A4 and resid 76 and name CB)	6.47	0.31	0.31
40	assign (segid 3A4 and resid 73 and name N)	(segid 3A4 and resid 76 and name N)	6.02	0.42	0.43
	assign (segid 3A4 and resid 73 and name O)	(segid 3A4 and resid 73 and name CB)	5.59	0.26	0.27
	assign (segid 3A4 and resid 73 and name O)	(segid 3A4 and resid 74 and name C)	3.16	0.09	0.09
	assign (segid 3A4 and resid 73 and name O)	(segid 3A4 and resid 74 and name CA)	3.09	0.23	0.23
	assign (segid 3A4 and resid 73 and name O)	(segid 3A4 and resid 74 and name CB)	2.78	0.04	0.03
45	assign (segid 3A4 and resid 73 and name O)	(segid 3A4 and resid 74 and name N)	4.22	0.08	0.08
	assign (segid 3A4 and resid 73 and name O)	(segid 3A4 and resid 74 and name O)	2.24	0.01	0.02
	assign (segid 3A4 and resid 73 and name O)	(segid 3A4 and resid 75 and name C)	3.61	0.34	0.34
	assign (segid 3A4 and resid 73 and name O)	(segid 3A4 and resid 75 and name CA)	4.33	0.43	0.42
	assign (segid 3A4 and resid 73 and name O)	(segid 3A4 and resid 75 and name CB)	4.52	0.34	0.34
50	assign (segid 3A4 and resid 73 and name O)	(segid 3A4 and resid 75 and name CG)	5.37	0.35	0.34
	assign (segid 3A4 and resid 73 and name O)	(segid 3A4 and resid 75 and name N)	6.53	0.38	0.38
	assign (segid 3A4 and resid 73 and name O)	(segid 3A4 and resid 75 and name O)	3.52	0.25	0.25
	assign (segid 3A4 and resid 73 and name O)	(segid 3A4 and resid 76 and name C)	5.15	0.28	0.28
	assign (segid 3A4 and resid 73 and name O)	(segid 3A4 and resid 76 and name CA)	4.49	0.58	0.58
55	assign (segid 3A4 and resid 73 and name O)	(segid 3A4 and resid 76 and name CB)	4.26	0.68	0.69
	assign (segid 3A4 and resid 73 and name O)	(segid 3A4 and resid 76 and name N)	4.11	0.76	0.76
	assign (segid 3A4 and resid 73 and name O)	(segid 3A4 and resid 76 and name O)	3.72	0.68	0.68
	assign (segid 3A4 and resid 73 and name O)	(segid 3A4 and resid 77 and name C)	5.66	0.56	0.55
	assign (segid 3A4 and resid 73 and name O)	(segid 3A4 and resid 77 and name CA)	5.65	0.50	0.51
60	assign (segid 3A4 and resid 73 and name O)	(segid 3A4 and resid 77 and name CB)	4.56	0.56	0.56
	assign (segid 3A4 and resid 73 and name O)	(segid 3A4 and resid 77 and name N)	4.16	0.65	0.64
	assign (segid 3A4 and resid 73 and name O)	(segid 3A4 and resid 77 and name O)	3.71	0.56	0.57
	assign (segid 3A4 and resid 73 and name O)	(segid 3A4 and resid 78 and name CA)	6.81	0.52	0.52
	assign (segid 3A4 and resid 73 and name O)	(segid 3A4 and resid 78 and name CB)	6.89	0.39	0.38
65	assign (segid 3A4 and resid 73 and name O)	(segid 3A4 and resid 78 and name N)	7.04	0.35	0.35
	assign (segid 3A4 and resid 73 and name O)	(segid 3A4 and resid 78 and name O)	5.57	0.43	0.42
	assign (segid 3A4 and resid 74 and name C)	(segid 3A4 and resid 74 and name CB)	2.50	0.02	0.01
	assign (segid 3A4 and resid 74 and name C)	(segid 3A4 and resid 74 and name O)	1.23	0.01	0.00
70	assign (segid 3A4 and resid 74 and name C)	(segid 3A4 and resid 75 and name C)	2.98	0.03	0.02
	assign (segid 3A4 and resid 74 and name C)	(segid 3A4 and resid 75 and name CA)	2.44	0.02	0.01
	assign (segid 3A4 and resid 74 and name C)	(segid 3A4 and resid 75 and name CB)	3.72	0.03	0.02
	assign (segid 3A4 and resid 74 and name C)	(segid 3A4 and resid 75 and name CG)	4.96	0.03	0.03
	assign (segid 3A4 and resid 74 and name C)	(segid 3A4 and resid 75 and name N)	1.33	0.01	0.01
	assign (segid 3A4 and resid 74 and name C)	(segid 3A4 and resid 75 and name O)	3.67	0.18	0.17
75	assign (segid 3A4 and resid 74 and name C)	(segid 3A4 and resid 76 and name C)	4.75	0.13	0.14
	assign (segid 3A4 and resid 74 and name C)	(segid 3A4 and resid 76 and name CA)	4.59	0.16	0.16
	assign (segid 3A4 and resid 74 and name C)	(segid 3A4 and resid 76 and name CB)	5.34	0.24	0.23
	assign (segid 3A4 and resid 74 and name C)	(segid 3A4 and resid 76 and name N)	3.41	0.21	0.20
	assign (segid 3A4 and resid 74 and name C)	(segid 3A4 and resid 76 and name O)	5.85	0.16	0.16
80	assign (segid 3A4 and resid 74 and name C)	(segid 3A4 and resid 77 and name C)	5.12	0.33	0.32
	assign (segid 3A4 and resid 74 and name C)	(segid 3A4 and resid 77 and name CA)	4.80	0.29	0.29
	assign (segid 3A4 and resid 74 and name C)	(segid 3A4 and resid 77 and name CB)	4.65	0.41	0.40
	assign (segid 3A4 and resid 74 and name C)	(segid 3A4 and resid 77 and name N)	4.04	0.20	0.19

	assign	(segid 3A4 and resid 74 and name C)	(segid 3A4 and resid 77 and name O)	6.34	0.34	0.33
	assign	(segid 3A4 and resid 74 and name C)	(segid 3A4 and resid 78 and name C)	6.16	0.37	0.36
	assign	(segid 3A4 and resid 74 and name C)	(segid 3A4 and resid 78 and name CA)	5.23	0.36	0.36
	assign	(segid 3A4 and resid 74 and name C)	(segid 3A4 and resid 78 and name CB)	4.82	0.40	0.39
5	assign	(segid 3A4 and resid 74 and name C)	(segid 3A4 and resid 78 and name N)	4.34	0.35	0.35
	assign	(segid 3A4 and resid 74 and name C)	(segid 3A4 and resid 79 and name CA)	7.09	0.30	0.29
	assign	(segid 3A4 and resid 74 and name C)	(segid 3A4 and resid 79 and name CB)	6.96	0.22	0.21
	assign	(segid 3A4 and resid 74 and name C)	(segid 3A4 and resid 79 and name N)	5.88	0.31	0.31
	assign	(segid 3A4 and resid 74 and name CA)	(segid 3A4 and resid 224 and name CA)	15.36	1.25	1.26
10	assign	(segid 3A4 and resid 74 and name CA)	(segid 3A4 and resid 224 and name CB)	14.96	1.31	1.30
	assign	(segid 3A4 and resid 74 and name CA)	(segid 3A4 and resid 225 and name CA)	17.38	1.20	1.20
	assign	(segid 3A4 and resid 74 and name CA)	(segid 3A4 and resid 240 and name CA)	12.62	1.74	1.74
	assign	(segid 3A4 and resid 74 and name CA)	(segid 3A4 and resid 240 and name CB)	12.20	1.84	1.83
	assign	(segid 3A4 and resid 74 and name CA)	(segid 3A4 and resid 241 and name CA)	15.27	1.73	1.72
15	assign	(segid 3A4 and resid 74 and name CA)	(segid 3A4 and resid 241 and name CB)	16.61	1.73	1.74
	assign	(segid 3A4 and resid 74 and name CA)	(segid 3A4 and resid 242 and name CA)	13.89	1.76	1.77
	assign	(segid 3A4 and resid 74 and name CA)	(segid 3A4 and resid 242 and name CB)	13.73	1.78	1.77
	assign	(segid 3A4 and resid 74 and name CA)	(segid 3A4 and resid 243 and name CA)	10.69	1.72	1.72
	assign	(segid 3A4 and resid 74 and name CA)	(segid 3A4 and resid 243 and name CB)	9.58	1.79	1.78
20	assign	(segid 3A4 and resid 74 and name CA)	(segid 3A4 and resid 244 and name CA)	13.16	1.63	1.63
	assign	(segid 3A4 and resid 74 and name CA)	(segid 3A4 and resid 244 and name CB)	14.18	1.62	1.63
	assign	(segid 3A4 and resid 74 and name CA)	(segid 3A4 and resid 245 and name CA)	15.47	1.60	1.59
	assign	(segid 3A4 and resid 74 and name CA)	(segid 3A4 and resid 245 and name CB)	16.16	1.66	1.66
	assign	(segid 3A4 and resid 74 and name CA)	(segid 3A4 and resid 246 and name CA)	13.28	1.43	1.44
25	assign	(segid 3A4 and resid 74 and name CA)	(segid 3A4 and resid 246 and name CB)	12.18	1.46	1.45
	assign	(segid 3A4 and resid 74 and name CA)	(segid 3A4 and resid 247 and name CA)	12.48	1.19	1.18
	assign	(segid 3A4 and resid 74 and name CA)	(segid 3A4 and resid 247 and name CB)	11.90	1.17	1.17
	assign	(segid 3A4 and resid 74 and name CA)	(segid 3A4 and resid 248 and name CA)	16.20	1.20	1.21
30	assign	(segid 3A4 and resid 74 and name CA)	(segid 3A4 and resid 248 and name CB)	17.03	1.29	1.30
	assign	(segid 3A4 and resid 74 and name CA)	(segid 3A4 and resid 249 and name CA)	17.19	1.25	1.26
	assign	(segid 3A4 and resid 74 and name CA)	(segid 3A4 and resid 250 and name CA)	15.40	1.08	1.07
	assign	(segid 3A4 and resid 74 and name CA)	(segid 3A4 and resid 250 and name CB)	13.94	1.06	1.06
	assign	(segid 3A4 and resid 74 and name CA)	(segid 3A4 and resid 251 and name CA)	16.98	0.98	0.97
	assign	(segid 3A4 and resid 74 and name CA)	(segid 3A4 and resid 251 and name CB)	16.88	0.94	0.95
35	assign	(segid 3A4 and resid 74 and name CA)	(segid 3A4 and resid 323 and name CA)	17.03	0.98	0.97
	assign	(segid 3A4 and resid 74 and name CA)	(segid 3A4 and resid 324 and name CB)	16.79	0.98	0.97
	assign	(segid 3A4 and resid 74 and name CA)	(segid 3A4 and resid 326 and name CB)	15.64	1.66	1.66
	assign	(segid 3A4 and resid 74 and name CA)	(segid 3A4 and resid 387 and name CA)	16.11	0.98	0.99
	assign	(segid 3A4 and resid 74 and name CA)	(segid 3A4 and resid 388 and name CA)	12.62	1.06	1.05
40	assign	(segid 3A4 and resid 74 and name CA)	(segid 3A4 and resid 388 and name CB)	11.61	1.28	1.29
	assign	(segid 3A4 and resid 74 and name CA)	(segid 3A4 and resid 389 and name CA)	12.63	0.49	0.50
	assign	(segid 3A4 and resid 74 and name CA)	(segid 3A4 and resid 390 and name CA)	15.90	0.38	0.38
	assign	(segid 3A4 and resid 74 and name CA)	(segid 3A4 and resid 390 and name CB)	16.59	0.54	0.54
45	assign	(segid 3A4 and resid 74 and name CA)	(segid 3A4 and resid 391 and name CA)	16.87	0.08	0.07
	assign	(segid 3A4 and resid 74 and name CA)	(segid 3A4 and resid 391 and name CB)	18.29	0.10	0.10
	assign	(segid 3A4 and resid 74 and name CA)	(segid 3A4 and resid 392 and name CA)	15.72	0.40	0.41
	assign	(segid 3A4 and resid 74 and name CA)	(segid 3A4 and resid 392 and name CB)	14.56	0.52	0.53
	assign	(segid 3A4 and resid 74 and name CA)	(segid 3A4 and resid 393 and name CA)	18.93	0.58	0.57
50	assign	(segid 3A4 and resid 74 and name CA)	(segid 3A4 and resid 74 and name C)	1.52	0.00	0.01
	assign	(segid 3A4 and resid 74 and name CA)	(segid 3A4 and resid 74 and name CB)	1.54	0.01	0.01
	assign	(segid 3A4 and resid 74 and name CA)	(segid 3A4 and resid 74 and name O)	2.40	0.04	0.03
	assign	(segid 3A4 and resid 74 and name CA)	(segid 3A4 and resid 75 and name C)	4.38	0.03	0.04
	assign	(segid 3A4 and resid 74 and name CA)	(segid 3A4 and resid 75 and name CA)	3.81	0.03	0.03
55	assign	(segid 3A4 and resid 74 and name CA)	(segid 3A4 and resid 75 and name CB)	4.85	0.08	0.08
	assign	(segid 3A4 and resid 74 and name CA)	(segid 3A4 and resid 75 and name CG)	6.23	0.05	0.05
	assign	(segid 3A4 and resid 74 and name CA)	(segid 3A4 and resid 75 and name N)	2.43	0.04	0.05
	assign	(segid 3A4 and resid 74 and name CA)	(segid 3A4 and resid 75 and name O)	5.12	0.19	0.20
	assign	(segid 3A4 and resid 74 and name CA)	(segid 3A4 and resid 76 and name C)	5.77	0.19	0.19
60	assign	(segid 3A4 and resid 74 and name CA)	(segid 3A4 and resid 76 and name CA)	5.63	0.19	0.19
	assign	(segid 3A4 and resid 74 and name CA)	(segid 3A4 and resid 76 and name CB)	6.07	0.30	0.30
	assign	(segid 3A4 and resid 74 and name CA)	(segid 3A4 and resid 76 and name N)	4.55	0.22	0.22
	assign	(segid 3A4 and resid 74 and name CA)	(segid 3A4 and resid 76 and name O)	6.90	0.22	0.22
	assign	(segid 3A4 and resid 74 and name CA)	(segid 3A4 and resid 77 and name C)	6.00	0.45	0.46
65	assign	(segid 3A4 and resid 74 and name CA)	(segid 3A4 and resid 77 and name CA)	5.48	0.42	0.42
	assign	(segid 3A4 and resid 74 and name CA)	(segid 3A4 and resid 77 and name CB)	4.92	0.58	0.59
	assign	(segid 3A4 and resid 74 and name CA)	(segid 3A4 and resid 77 and name N)	4.87	0.29	0.29
	assign	(segid 3A4 and resid 74 and name CA)	(segid 3A4 and resid 78 and name CA)	6.33	0.47	0.48
	assign	(segid 3A4 and resid 74 and name CA)	(segid 3A4 and resid 78 and name CB)	5.93	0.50	0.49
70	assign	(segid 3A4 and resid 74 and name CA)	(segid 3A4 and resid 78 and name N)	5.38	0.47	0.47
	assign	(segid 3A4 and resid 74 and name CA)	(segid 3A4 and resid 79 and name CA)	8.51	0.33	0.32
	assign	(segid 3A4 and resid 74 and name CA)	(segid 3A4 and resid 79 and name CB)	8.41	0.22	0.22
	assign	(segid 3A4 and resid 74 and name CA)	(segid 3A4 and resid 80 and name CA)	10.08	0.35	0.35
	assign	(segid 3A4 and resid 74 and name CA)	(segid 3A4 and resid 81 and name CA)	11.20	0.55	0.55
75	assign	(segid 3A4 and resid 74 and name CA)	(segid 3A4 and resid 81 and name CB)	10.59	0.64	0.64
	assign	(segid 3A4 and resid 74 and name CA)	(segid 3A4 and resid 82 and name CA)	12.86	0.75	0.75
	assign	(segid 3A4 and resid 74 and name CA)	(segid 3A4 and resid 82 and name CB)	12.47	0.95	0.95
	assign	(segid 3A4 and resid 74 and name CA)	(segid 3A4 and resid 83 and name CA)	14.22	0.39	0.39
	assign	(segid 3A4 and resid 74 and name CA)	(segid 3A4 and resid 83 and name CB)	13.67	0.38	0.39
80	assign	(segid 3A4 and resid 74 and name CA)	(segid 3A4 and resid 84 and name CA)	16.64	0.53	0.53
	assign	(segid 3A4 and resid 74 and name CA)	(segid 3A4 and resid 84 and name CB)	16.52	0.71	0.70
	assign	(segid 3A4 and resid 74 and name CA)	(segid 3A4 and resid 85 and name CA)	18.11	0.93	0.93
	assign	(segid 3A4 and resid 74 and name CA)	(segid 3A4 and resid 85 and name CB)	17.66	1.12	1.12

	assign (segid 3A4 and resid 74 and name CA) (segid 3A4 and resid 86 and name CA)	18.43	0.68	0.68
	assign (segid 3A4 and resid 74 and name CA) (segid 3A4 and resid 86 and name CB)	17.56	0.78	0.78
	assign (segid 3A4 and resid 74 and name CB) (segid 3A4 and resid 224 and name CA)	15.60	1.45	1.16
	assign (segid 3A4 and resid 74 and name CB) (segid 3A4 and resid 224 and name CB)	15.09	1.52	1.51
5	assign (segid 3A4 and resid 74 and name CB) (segid 3A4 and resid 225 and name CA)	17.46	1.39	1.39
	assign (segid 3A4 and resid 74 and name CB) (segid 3A4 and resid 240 and name CA)	12.16	1.89	1.88
	assign (segid 3A4 and resid 74 and name CB) (segid 3A4 and resid 240 and name CB)	11.60	1.95	1.96
	assign (segid 3A4 and resid 74 and name CB) (segid 3A4 and resid 241 and name CA)	14.65	1.94	1.95
	assign (segid 3A4 and resid 74 and name CB) (segid 3A4 and resid 241 and name CB)	15.96	1.95	1.95
10	assign (segid 3A4 and resid 74 and name CB) (segid 3A4 and resid 242 and name CA)	13.00	2.00	1.99
	assign (segid 3A4 and resid 74 and name CB) (segid 3A4 and resid 242 and name CB)	12.73	1.98	1.98
	assign (segid 3A4 and resid 74 and name CB) (segid 3A4 and resid 243 and name CA)	9.96	1.98	1.99
	assign (segid 3A4 and resid 74 and name CB) (segid 3A4 and resid 243 and name CB)	8.94	2.04	2.04
	assign (segid 3A4 and resid 74 and name CB) (segid 3A4 and resid 244 and name CA)	12.74	1.90	1.90
15	assign (segid 3A4 and resid 74 and name CB) (segid 3A4 and resid 244 and name CB)	13.81	1.89	1.89
	assign (segid 3A4 and resid 74 and name CB) (segid 3A4 and resid 245 and name CA)	14.78	1.87	1.87
	assign (segid 3A4 and resid 74 and name CB) (segid 3A4 and resid 245 and name CB)	15.37	1.94	1.94
	assign (segid 3A4 and resid 74 and name CB) (segid 3A4 and resid 246 and name CA)	12.48	1.68	1.69
	assign (segid 3A4 and resid 74 and name CB) (segid 3A4 and resid 246 and name CB)	11.29	1.70	1.70
20	assign (segid 3A4 and resid 74 and name CB) (segid 3A4 and resid 247 and name CA)	12.08	1.42	1.42
	assign (segid 3A4 and resid 74 and name CB) (segid 3A4 and resid 247 and name CB)	11.64	1.40	1.40
	assign (segid 3A4 and resid 74 and name CB) (segid 3A4 and resid 248 and name CA)	15.83	1.47	1.46
	assign (segid 3A4 and resid 74 and name CB) (segid 3A4 and resid 248 and name CB)	16.63	1.58	1.57
	assign (segid 3A4 and resid 74 and name CB) (segid 3A4 and resid 249 and name CA)	16.58	1.50	1.49
25	assign (segid 3A4 and resid 74 and name CB) (segid 3A4 and resid 250 and name CA)	14.92	1.26	1.26
	assign (segid 3A4 and resid 74 and name CB) (segid 3A4 and resid 250 and name CB)	13.49	1.23	1.24
	assign (segid 3A4 and resid 74 and name CB) (segid 3A4 and resid 251 and name CA)	16.79	1.17	1.17
	assign (segid 3A4 and resid 74 and name CB) (segid 3A4 and resid 251 and name CB)	16.77	1.15	1.15
	assign (segid 3A4 and resid 74 and name CB) (segid 3A4 and resid 324 and name CB)	16.24	1.24	1.23
30	assign (segid 3A4 and resid 74 and name CB) (segid 3A4 and resid 387 and name CA)	16.77	1.10	1.10
	assign (segid 3A4 and resid 74 and name CB) (segid 3A4 and resid 388 and name CA)	13.38	1.18	1.17
	assign (segid 3A4 and resid 74 and name CB) (segid 3A4 and resid 388 and name CB)	12.40	1.44	1.44
	assign (segid 3A4 and resid 74 and name CB) (segid 3A4 and resid 389 and name CA)	13.09	0.60	0.59
	assign (segid 3A4 and resid 74 and name CB) (segid 3A4 and resid 389 and name CB)	12.95	0.65	0.64
35	assign (segid 3A4 and resid 74 and name CB) (segid 3A4 and resid 390 and name CA)	16.42	0.40	0.40
	assign (segid 3A4 and resid 74 and name CB) (segid 3A4 and resid 390 and name CB)	17.22	0.54	0.54
	assign (segid 3A4 and resid 74 and name CB) (segid 3A4 and resid 391 and name CA)	17.26	0.10	0.10
	assign (segid 3A4 and resid 74 and name CB) (segid 3A4 and resid 391 and name CB)	18.64	0.14	0.14
	assign (segid 3A4 and resid 74 and name CB) (segid 3A4 and resid 392 and name CA)	16.25	0.48	0.49
40	assign (segid 3A4 and resid 74 and name CB) (segid 3A4 and resid 392 and name CB)	15.06	0.62	0.62
	assign (segid 3A4 and resid 74 and name CB) (segid 3A4 and resid 75 and name C)	5.39	0.06	0.06
	assign (segid 3A4 and resid 74 and name CB) (segid 3A4 and resid 75 and name CB)	4.49	0.11	0.11
	assign (segid 3A4 and resid 74 and name CB) (segid 3A4 and resid 75 and name CB)	5.40	0.20	0.20
	assign (segid 3A4 and resid 74 and name CB) (segid 3A4 and resid 75 and name CG)	6.80	0.18	0.17
45	assign (segid 3A4 and resid 74 and name CB) (segid 3A4 and resid 75 and name N)	3.18	0.14	0.14
	assign (segid 3A4 and resid 74 and name CB) (segid 3A4 and resid 75 and name O)	6.06	0.15	0.15
	assign (segid 3A4 and resid 74 and name CB) (segid 3A4 and resid 76 and name C)	7.13	0.16	0.16
	assign (segid 3A4 and resid 74 and name CB) (segid 3A4 and resid 76 and name CA)	6.98	0.19	0.19
	assign (segid 3A4 and resid 74 and name CB) (segid 3A4 and resid 76 and name CB)	7.51	0.30	0.31
50	assign (segid 3A4 and resid 74 and name CB) (segid 3A4 and resid 76 and name N)	5.79	0.24	0.24
	assign (segid 3A4 and resid 74 and name CB) (segid 3A4 and resid 77 and name CA)	6.75	0.41	0.41
	assign (segid 3A4 and resid 74 and name CB) (segid 3A4 and resid 77 and name CB)	6.13	0.57	0.58
	assign (segid 3A4 and resid 74 and name CB) (segid 3A4 and resid 77 and name N)	6.24	0.25	0.26
	assign (segid 3A4 and resid 74 and name CB) (segid 3A4 and resid 78 and name CA)	6.97	0.51	0.51
55	assign (segid 3A4 and resid 74 and name CB) (segid 3A4 and resid 78 and name CB)	6.26	0.55	0.55
	assign (segid 3A4 and resid 74 and name CB) (segid 3A4 and resid 78 and name N)	6.26	0.47	0.47
	assign (segid 3A4 and resid 74 and name CB) (segid 3A4 and resid 79 and name CA)	9.35	0.34	0.33
	assign (segid 3A4 and resid 74 and name CB) (segid 3A4 and resid 79 and name CB)	9.31	0.22	0.22
	assign (segid 3A4 and resid 74 and name CB) (segid 3A4 and resid 80 and name CA)	11.23	0.34	0.34
60	assign (segid 3A4 and resid 74 and name CB) (segid 3A4 and resid 81 and name CA)	12.05	0.59	0.60
	assign (segid 3A4 and resid 74 and name CB) (segid 3A4 and resid 81 and name CB)	11.32	0.68	0.69
	assign (segid 3A4 and resid 74 and name CB) (segid 3A4 and resid 82 and name CA)	13.50	0.86	0.87
	assign (segid 3A4 and resid 74 and name CB) (segid 3A4 and resid 82 and name CB)	13.00	1.06	1.06
65	assign (segid 3A4 and resid 74 and name CB) (segid 3A4 and resid 83 and name CA)	15.11	0.43	0.44
	assign (segid 3A4 and resid 74 and name CB) (segid 3A4 and resid 83 and name CB)	14.67	0.38	0.37
	assign (segid 3A4 and resid 74 and name CB) (segid 3A4 and resid 84 and name CA)	17.58	0.60	0.61
	assign (segid 3A4 and resid 74 and name CB) (segid 3A4 and resid 84 and name CB)	17.50	0.76	0.75
	assign (segid 3A4 and resid 74 and name CB) (segid 3A4 and resid 86 and name CB)	18.14	0.88	0.89
	assign (segid 3A4 and resid 74 and name N) (segid 3A4 and resid 74 and name C)	2.46	0.01	0.01
70	assign (segid 3A4 and resid 74 and name N) (segid 3A4 and resid 74 and name CA)	1.46	0.01	0.00
	assign (segid 3A4 and resid 74 and name N) (segid 3A4 and resid 74 and name CB)	2.46	0.03	0.03
	assign (segid 3A4 and resid 74 and name N) (segid 3A4 and resid 74 and name O)	3.50	0.04	0.04
	assign (segid 3A4 and resid 74 and name N) (segid 3A4 and resid 75 and name C)	4.74	0.05	0.05
	assign (segid 3A4 and resid 74 and name N) (segid 3A4 and resid 75 and name CA)	4.20	0.06	0.05
75	assign (segid 3A4 and resid 74 and name N) (segid 3A4 and resid 75 and name CB)	4.89	0.11	0.11
	assign (segid 3A4 and resid 74 and name N) (segid 3A4 and resid 75 and name CG)	6.31	0.11	0.11
	assign (segid 3A4 and resid 74 and name N) (segid 3A4 and resid 75 and name N)	2.78	0.05	0.05
	assign (segid 3A4 and resid 74 and name N) (segid 3A4 and resid 75 and name O)	5.70	0.15	0.14
	assign (segid 3A4 and resid 74 and name N) (segid 3A4 and resid 76 and name C)	6.01	0.20	0.21
	assign (segid 3A4 and resid 74 and name N) (segid 3A4 and resid 76 and name CA)	5.62	0.24	0.23
80	assign (segid 3A4 and resid 74 and name N) (segid 3A4 and resid 76 and name CB)	5.72	0.36	0.37
	assign (segid 3A4 and resid 74 and name N) (segid 3A4 and resid 76 and name N)	4.57	0.23	0.24
	assign (segid 3A4 and resid 74 and name N) (segid 3A4 and resid 76 and name O)	7.22	0.21	0.21

	assign (segid 3A4 and resid 74 and name N) (segid 3A4 and resid 77 and name C)	6.84	0.44	0.43
	assign (segid 3A4 and resid 74 and name N) (segid 3A4 and resid 77 and name CA)	6.06	0.44	0.45
	assign (segid 3A4 and resid 74 and name N) (segid 3A4 and resid 77 and name CB)	5.55	0.63	0.63
	assign (segid 3A4 and resid 74 and name N) (segid 3A4 and resid 77 and name N)	5.25	0.32	0.32
5	assign (segid 3A4 and resid 74 and name N) (segid 3A4 and resid 78 and name N)	6.37	0.41	0.42
	assign (segid 3A4 and resid 74 and name O) (segid 3A4 and resid 74 and name CB)	3.26	0.13	0.13
	assign (segid 3A4 and resid 74 and name O) (segid 3A4 and resid 75 and name C)	2.87	0.04	0.05
	assign (segid 3A4 and resid 74 and name O) (segid 3A4 and resid 75 and name CA)	2.77	0.03	0.02
	assign (segid 3A4 and resid 74 and name O) (segid 3A4 and resid 75 and name CB)	4.26	0.02	0.01
10	assign (segid 3A4 and resid 74 and name O) (segid 3A4 and resid 75 and name CG)	5.26	0.09	0.09
	assign (segid 3A4 and resid 74 and name O) (segid 3A4 and resid 75 and name N)	2.25	0.01	0.01
	assign (segid 3A4 and resid 74 and name O) (segid 3A4 and resid 75 and name O)	3.16	0.21	0.21
	assign (segid 3A4 and resid 74 and name O) (segid 3A4 and resid 76 and name C)	4.25	0.20	0.21
	assign (segid 3A4 and resid 74 and name O) (segid 3A4 and resid 76 and name CA)	4.43	0.23	0.23
15	assign (segid 3A4 and resid 74 and name O) (segid 3A4 and resid 76 and name CB)	5.39	0.29	0.28
	assign (segid 3A4 and resid 74 and name O) (segid 3A4 and resid 76 and name N)	3.47	0.26	0.26
	assign (segid 3A4 and resid 74 and name O) (segid 3A4 and resid 76 and name O)	5.22	0.22	0.22
	assign (segid 3A4 and resid 74 and name O) (segid 3A4 and resid 77 and name C)	4.08	0.33	0.32
	assign (segid 3A4 and resid 74 and name O) (segid 3A4 and resid 77 and name CA)	3.99	0.28	0.28
20	assign (segid 3A4 and resid 74 and name O) (segid 3A4 and resid 77 and name CB)	3.94	0.34	0.33
	assign (segid 3A4 and resid 74 and name O) (segid 3A4 and resid 77 and name N)	3.45	0.24	0.24
	assign (segid 3A4 and resid 74 and name O) (segid 3A4 and resid 77 and name O)	5.26	0.33	0.34
	assign (segid 3A4 and resid 74 and name O) (segid 3A4 and resid 78 and name C)	5.08	0.43	0.43
	assign (segid 3A4 and resid 74 and name O) (segid 3A4 and resid 78 and name CA)	4.07	0.42	0.41
25	assign (segid 3A4 and resid 74 and name O) (segid 3A4 and resid 78 and name CB)	3.74	0.45	0.45
	assign (segid 3A4 and resid 74 and name O) (segid 3A4 and resid 78 and name N)	3.21	0.37	0.37
	assign (segid 3A4 and resid 74 and name O) (segid 3A4 and resid 78 and name O)	6.24	0.45	0.44
	assign (segid 3A4 and resid 74 and name O) (segid 3A4 and resid 79 and name CA)	6.25	0.37	0.37
	assign (segid 3A4 and resid 74 and name O) (segid 3A4 and resid 79 and name CB)	6.34	0.29	0.30
30	assign (segid 3A4 and resid 74 and name O) (segid 3A4 and resid 79 and name N)	4.95	0.39	0.38
	assign (segid 3A4 and resid 74 and name O) (segid 3A4 and resid 80 and name N)	6.92	0.36	0.36
	assign (segid 3A4 and resid 75 and name C) (segid HEM and resid 1 and name OLD)	6.91	0.32	0.31
	assign (segid 3A4 and resid 75 and name C) (segid 3A4 and resid 75 and name CB)	2.52	0.02	0.02
35	assign (segid 3A4 and resid 75 and name C) (segid 3A4 and resid 75 and name CG)	2.96	0.11	0.12
	assign (segid 3A4 and resid 75 and name C) (segid 3A4 and resid 75 and name O)	1.24	0.01	0.00
	assign (segid 3A4 and resid 75 and name C) (segid 3A4 and resid 76 and name C)	3.04	0.08	0.08
	assign (segid 3A4 and resid 75 and name C) (segid 3A4 and resid 76 and name CA)	2.45	0.02	0.03
	assign (segid 3A4 and resid 75 and name C) (segid 3A4 and resid 76 and name CB)	3.72	0.02	0.02
40	assign (segid 3A4 and resid 75 and name C) (segid 3A4 and resid 76 and name N)	1.33	0.00	0.01
	assign (segid 3A4 and resid 75 and name C) (segid 3A4 and resid 76 and name O)	3.94	0.10	0.10
	assign (segid 3A4 and resid 75 and name C) (segid 3A4 and resid 77 and name C)	4.55	0.13	0.12
	assign (segid 3A4 and resid 75 and name C) (segid 3A4 and resid 77 and name CA)	4.42	0.15	0.14
	assign (segid 3A4 and resid 75 and name C) (segid 3A4 and resid 77 and name CB)	5.17	0.20	0.20
	assign (segid 3A4 and resid 75 and name C) (segid 3A4 and resid 77 and name N)	3.22	0.13	0.14
45	assign (segid 3A4 and resid 75 and name C) (segid 3A4 and resid 77 and name O)	5.60	0.16	0.16
	assign (segid 3A4 and resid 75 and name C) (segid 3A4 and resid 78 and name C)	4.87	0.07	0.07
	assign (segid 3A4 and resid 75 and name C) (segid 3A4 and resid 78 and name CA)	4.68	0.07	0.07
	assign (segid 3A4 and resid 75 and name C) (segid 3A4 and resid 78 and name CB)	4.68	0.17	0.17
50	assign (segid 3A4 and resid 75 and name C) (segid 3A4 and resid 78 and name N)	3.90	0.06	0.06
	assign (segid 3A4 and resid 75 and name C) (segid 3A4 and resid 78 and name O)	6.06	0.09	0.08
	assign (segid 3A4 and resid 75 and name C) (segid 3A4 and resid 79 and name C)	5.87	0.11	0.11
	assign (segid 3A4 and resid 75 and name C) (segid 3A4 and resid 79 and name CA)	4.82	0.10	0.10
	assign (segid 3A4 and resid 75 and name C) (segid 3A4 and resid 79 and name CB)	4.28	0.11	0.12
	assign (segid 3A4 and resid 75 and name C) (segid 3A4 and resid 79 and name CG)	5.59	0.10	0.11
55	assign (segid 3A4 and resid 75 and name C) (segid 3A4 and resid 79 and name N)	4.01	0.07	0.08
	assign (segid 3A4 and resid 75 and name C) (segid 3A4 and resid 79 and name O)	7.05	0.12	0.13
	assign (segid 3A4 and resid 75 and name C) (segid 3A4 and resid 80 and name CA)	6.97	0.18	0.17
	assign (segid 3A4 and resid 75 and name C) (segid 3A4 and resid 80 and name N)	5.71	0.15	0.16
60	assign (segid 3A4 and resid 75 and name CA) (segid 3A4 and resid 220 and name CA)	17.89	0.87	0.88
	assign (segid 3A4 and resid 75 and name CA) (segid 3A4 and resid 220 and name CB)	17.22	0.91	0.92
	assign (segid 3A4 and resid 75 and name CA) (segid 3A4 and resid 221 and name CA)	18.29	0.69	0.69
	assign (segid 3A4 and resid 75 and name CA) (segid 3A4 and resid 223 and name CA)	17.82	0.74	0.75
	assign (segid 3A4 and resid 75 and name CA) (segid 3A4 and resid 223 and name CB)	17.40	0.85	0.86
65	assign (segid 3A4 and resid 75 and name CA) (segid 3A4 and resid 224 and name CA)	15.04	0.64	0.65
	assign (segid 3A4 and resid 75 and name CA) (segid 3A4 and resid 224 and name CB)	14.51	0.63	0.63
	assign (segid 3A4 and resid 75 and name CA) (segid 3A4 and resid 225 and name CA)	17.69	0.70	0.70
	assign (segid 3A4 and resid 75 and name CA) (segid 3A4 and resid 240 and name CA)	14.37	1.05	1.06
	assign (segid 3A4 and resid 75 and name CA) (segid 3A4 and resid 240 and name CB)	14.16	1.15	1.16
70	assign (segid 3A4 and resid 75 and name CA) (segid 3A4 and resid 241 and name CA)	16.47	0.97	0.97
	assign (segid 3A4 and resid 75 and name CA) (segid 3A4 and resid 242 and name CA)	14.95	1.08	1.08
	assign (segid 3A4 and resid 75 and name CA) (segid 3A4 and resid 242 and name CB)	15.03	1.15	1.14
	assign (segid 3A4 and resid 75 and name CA) (segid 3A4 and resid 243 and name CA)	11.41	1.04	1.05
	assign (segid 3A4 and resid 75 and name CA) (segid 3A4 and resid 243 and name CB)	10.56	1.11	1.11
75	assign (segid 3A4 and resid 75 and name CA) (segid 3A4 and resid 244 and name CA)	13.29	0.93	0.93
	assign (segid 3A4 and resid 75 and name CA) (segid 3A4 and resid 244 and name CB)	14.48	0.91	0.91
	assign (segid 3A4 and resid 75 and name CA) (segid 3A4 and resid 245 and name CA)	15.33	0.91	0.91
	assign (segid 3A4 and resid 75 and name CA) (segid 3A4 and resid 245 and name CB)	16.25	0.97	0.96
	assign (segid 3A4 and resid 75 and name CA) (segid 3A4 and resid 246 and name CA)	12.74	0.86	0.85
	assign (segid 3A4 and resid 75 and name CA) (segid 3A4 and resid 246 and name CB)	11.84	0.87	0.87
80	assign (segid 3A4 and resid 75 and name CA) (segid 3A4 and resid 247 and name CA)	11.23	0.66	0.66
	assign (segid 3A4 and resid 75 and name CA) (segid 3A4 and resid 247 and name CB)	10.76	0.61	0.62
	assign (segid 3A4 and resid 75 and name CA) (segid 3A4 and resid 248 and name CA)	14.91	0.62	0.62
	assign (segid 3A4 and resid 75 and name CA) (segid 3A4 and resid 248 and name CB)	15.99	0.66	0.65

	assign (segid 3A4 and resid 75 and name CA) (segid 3A4 and resid 249 and name CA)	15.77	0.77	0.71
	assign (segid 3A4 and resid 75 and name CA) (segid 3A4 and resid 250 and name CA)	13.31	0.63	0.64
	assign (segid 3A4 and resid 75 and name CA) (segid 3A4 and resid 250 and name CB)	11.81	0.65	0.66
	assign (segid 3A4 and resid 75 and name CA) (segid 3A4 and resid 251 and name CA)	14.62	0.52	0.52
5	assign (segid 3A4 and resid 75 and name CA) (segid 3A4 and resid 251 and name CB)	14.65	0.47	0.48
	assign (segid 3A4 and resid 75 and name CA) (segid 3A4 and resid 252 and name CA)	18.09	0.56	0.56
	assign (segid 3A4 and resid 75 and name CA) (segid 3A4 and resid 252 and name CB)	18.68	0.57	0.58
	assign (segid 3A4 and resid 75 and name CA) (segid 3A4 and resid 253 and name CA)	18.03	0.66	0.67
	assign (segid 3A4 and resid 75 and name CA) (segid 3A4 and resid 254 and name CA)	16.28	0.58	0.59
10	assign (segid 3A4 and resid 75 and name CA) (segid 3A4 and resid 322 and name CA)	16.03	0.51	0.51
	assign (segid 3A4 and resid 75 and name CA) (segid 3A4 and resid 323 and name CA)	14.75	0.75	0.75
	assign (segid 3A4 and resid 75 and name CA) (segid 3A4 and resid 323 and name CB)	14.89	0.88	0.88
	assign (segid 3A4 and resid 75 and name CA) (segid 3A4 and resid 324 and name CA)	15.78	0.92	0.91
	assign (segid 3A4 and resid 75 and name CA) (segid 3A4 and resid 324 and name CB)	15.42	0.86	0.87
15	assign (segid 3A4 and resid 75 and name CA) (segid 3A4 and resid 325 and name CA)	17.25	1.21	1.21
	assign (segid 3A4 and resid 75 and name CA) (segid 3A4 and resid 326 and name CA)	16.13	1.25	1.26
	assign (segid 3A4 and resid 75 and name CA) (segid 3A4 and resid 326 and name CB)	15.03	1.39	1.39
	assign (segid 3A4 and resid 75 and name CA) (segid 3A4 and resid 384 and name CA)	17.50	0.21	0.22
	assign (segid 3A4 and resid 75 and name CA) (segid 3A4 and resid 384 and name CB)	17.54	0.18	0.19
20	assign (segid 3A4 and resid 75 and name CA) (segid 3A4 and resid 385 and name CA)	15.89	0.52	0.52
	assign (segid 3A4 and resid 75 and name CA) (segid 3A4 and resid 386 and name CA)	15.21	0.59	0.59
	assign (segid 3A4 and resid 75 and name CA) (segid 3A4 and resid 387 and name CA)	12.80	0.68	0.69
	assign (segid 3A4 and resid 75 and name CA) (segid 3A4 and resid 388 and name CA)	9.28	0.82	0.83
	assign (segid 3A4 and resid 75 and name CA) (segid 3A4 and resid 388 and name CB)	8.48	1.01	1.02
25	assign (segid 3A4 and resid 75 and name CA) (segid 3A4 and resid 389 and name CA)	8.94	0.41	0.40
	assign (segid 3A4 and resid 75 and name CA) (segid 3A4 and resid 389 and name CB)	9.02	0.39	0.39
	assign (segid 3A4 and resid 75 and name CA) (segid 3A4 and resid 390 and name CA)	12.18	0.34	0.34
	assign (segid 3A4 and resid 75 and name CA) (segid 3A4 and resid 390 and name CB)	12.93	0.46	0.46
	assign (segid 3A4 and resid 75 and name CA) (segid 3A4 and resid 391 and name CA)	13.20	0.08	0.09
30	assign (segid 3A4 and resid 75 and name CA) (segid 3A4 and resid 391 and name CB)	14.64	0.07	0.08
	assign (segid 3A4 and resid 75 and name CA) (segid 3A4 and resid 392 and name CA)	12.29	0.26	0.26
	assign (segid 3A4 and resid 75 and name CA) (segid 3A4 and resid 392 and name CB)	11.23	0.33	0.33
	assign (segid 3A4 and resid 75 and name CA) (segid 3A4 and resid 393 and name CA)	15.63	0.30	0.29
	assign (segid 3A4 and resid 75 and name CA) (segid 3A4 and resid 394 and name CA)	17.72	0.21	0.21
35	assign (segid 3A4 and resid 75 and name CA) (segid 3A4 and resid 394 and name CB)	17.41	0.22	0.22
	assign (segid 3A4 and resid 75 and name CA) (segid HEM and resid 1 and name CGD)	7.54	0.13	0.13
	assign (segid 3A4 and resid 75 and name CA) (segid HEM and resid 1 and name OLD)	6.91	0.18	0.17
	assign (segid 3A4 and resid 75 and name CA) (segid HEM and resid 1 and name O2D)	7.38	0.24	0.24
	assign (segid 3A4 and resid 75 and name CA) (segid 3A4 and resid 75 and name C)	1.52	0.01	0.01
40	assign (segid 3A4 and resid 75 and name CA) (segid 3A4 and resid 75 and name CB)	1.54	0.01	0.01
	assign (segid 3A4 and resid 75 and name CA) (segid 3A4 and resid 75 and name CG)	2.56	0.04	0.04
	assign (segid 3A4 and resid 75 and name CA) (segid 3A4 and resid 75 and name O)	2.40	0.02	0.02
	assign (segid 3A4 and resid 75 and name CA) (segid 3A4 and resid 76 and name C)	4.48	0.06	0.07
	assign (segid 3A4 and resid 75 and name CA) (segid 3A4 and resid 76 and name CA)	3.82	0.02	0.03
45	assign (segid 3A4 and resid 75 and name CA) (segid 3A4 and resid 76 and name CB)	4.87	0.04	0.03
	assign (segid 3A4 and resid 75 and name CA) (segid 3A4 and resid 76 and name N)	2.44	0.02	0.02
	assign (segid 3A4 and resid 75 and name CA) (segid 3A4 and resid 76 and name O)	5.43	0.09	0.10
	assign (segid 3A4 and resid 75 and name CA) (segid 3A4 and resid 77 and name C)	5.62	0.15	0.14
	assign (segid 3A4 and resid 75 and name CA) (segid 3A4 and resid 77 and name CA)	5.54	0.16	0.15
50	assign (segid 3A4 and resid 75 and name CA) (segid 3A4 and resid 77 and name CB)	6.00	0.25	0.25
	assign (segid 3A4 and resid 75 and name CA) (segid 3A4 and resid 77 and name N)	4.43	0.13	0.13
	assign (segid 3A4 and resid 75 and name CA) (segid 3A4 and resid 77 and name O)	6.73	0.17	0.17
	assign (segid 3A4 and resid 75 and name CA) (segid 3A4 and resid 78 and name C)	5.73	0.15	0.15
	assign (segid 3A4 and resid 75 and name CA) (segid 3A4 and resid 78 and name CA)	5.36	0.12	0.13
55	assign (segid 3A4 and resid 75 and name CA) (segid 3A4 and resid 78 and name CB)	4.94	0.22	0.22
	assign (segid 3A4 and resid 75 and name CA) (segid 3A4 and resid 78 and name N)	4.75	0.10	0.10
	assign (segid 3A4 and resid 75 and name CA) (segid 3A4 and resid 78 and name O)	6.91	0.18	0.18
	assign (segid 3A4 and resid 75 and name CA) (segid 3A4 and resid 79 and name C)	7.10	0.16	0.15
	assign (segid 3A4 and resid 75 and name CA) (segid 3A4 and resid 79 and name CA)	5.88	0.15	0.16
60	assign (segid 3A4 and resid 75 and name CA) (segid 3A4 and resid 79 and name CB)	5.35	0.14	0.15
	assign (segid 3A4 and resid 75 and name CA) (segid 3A4 and resid 79 and name CG)	6.62	0.14	0.13
	assign (segid 3A4 and resid 75 and name CA) (segid 3A4 and resid 79 and name N)	5.03	0.14	0.14
	assign (segid 3A4 and resid 75 and name CA) (segid 3A4 and resid 80 and name CA)	8.38	0.20	0.20
	assign (segid 3A4 and resid 75 and name CA) (segid 3A4 and resid 80 and name N)	7.08	0.19	0.18
65	assign (segid 3A4 and resid 75 and name CA) (segid 3A4 and resid 81 and name CA)	10.13	0.19	0.19
	assign (segid 3A4 and resid 75 and name CA) (segid 3A4 and resid 81 and name CB)	9.88	0.20	0.19
	assign (segid 3A4 and resid 75 and name CA) (segid 3A4 and resid 82 and name CA)	10.90	0.52	0.53
	assign (segid 3A4 and resid 75 and name CA) (segid 3A4 and resid 82 and name CB)	10.33	0.80	0.80
	assign (segid 3A4 and resid 75 and name CA) (segid 3A4 and resid 83 and name CA)	11.74	0.18	0.18
70	assign (segid 3A4 and resid 75 and name CA) (segid 3A4 and resid 83 and name CB)	11.15	0.27	0.27
	assign (segid 3A4 and resid 75 and name CA) (segid 3A4 and resid 84 and name CA)	14.67	0.36	0.37
	assign (segid 3A4 and resid 75 and name CA) (segid 3A4 and resid 84 and name CB)	14.83	0.57	0.57
	assign (segid 3A4 and resid 75 and name CA) (segid 3A4 and resid 85 and name CA)	16.13	0.52	0.53
	assign (segid 3A4 and resid 75 and name CA) (segid 3A4 and resid 85 and name CB)	15.85	0.67	0.66
75	assign (segid 3A4 and resid 75 and name CA) (segid 3A4 and resid 86 and name CA)	15.85	0.29	0.28
	assign (segid 3A4 and resid 75 and name CA) (segid 3A4 and resid 86 and name CB)	14.84	0.42	0.43
	assign (segid 3A4 and resid 75 and name CB) (segid 3A4 and resid 220 and name CB)	18.11	0.77	0.76
	assign (segid 3A4 and resid 75 and name CB) (segid 3A4 and resid 224 and name CA)	16.32	0.59	0.59
80	assign (segid 3A4 and resid 75 and name CB) (segid 3A4 and resid 224 and name CB)	15.74	0.58	0.57
	assign (segid 3A4 and resid 75 and name CB) (segid 3A4 and resid 240 and name CA)	15.75	1.05	1.05
	assign (segid 3A4 and resid 75 and name CB) (segid 3A4 and resid 240 and name CB)	15.50	1.16	1.16
	assign (segid 3A4 and resid 75 and name CB) (segid 3A4 and resid 241 and name CA)	17.75	0.96	0.95
	assign (segid 3A4 and resid 75 and name CB) (segid 3A4 and resid 242 and name CA)	16.04	1.10	1.10

5	assign	(segid 3A4 and resid 75 and name CB)	(segid 3A4 and resid 242 and name CB)	16.08	1.18	1.18
	assign	(segid 3A4 and resid 75 and name CB)	(segid 3A4 and resid 243 and name CA)	12.57	1.05	1.05
	assign	(segid 3A4 and resid 75 and name CB)	(segid 3A4 and resid 243 and name CB)	11.81	1.12	1.12
	assign	(segid 3A4 and resid 75 and name CB)	(segid 3A4 and resid 244 and name CA)	14.48	0.88	0.89
	assign	(segid 3A4 and resid 75 and name CB)	(segid 3A4 and resid 244 and name CB)	15.73	0.87	0.86
	assign	(segid 3A4 and resid 75 and name CB)	(segid 3A4 and resid 245 and name CA)	16.30	0.87	0.87
	assign	(segid 3A4 and resid 75 and name CB)	(segid 3A4 and resid 245 and name CB)	17.21	0.95	0.94
	assign	(segid 3A4 and resid 75 and name CB)	(segid 3A4 and resid 246 and name CA)	13.48	0.84	0.85
	assign	(segid 3A4 and resid 75 and name CB)	(segid 3A4 and resid 246 and name CB)	12.57	0.88	0.89
10	assign	(segid 3A4 and resid 75 and name CB)	(segid 3A4 and resid 247 and name CA)	12.03	0.60	0.59
	assign	(segid 3A4 and resid 75 and name CB)	(segid 3A4 and resid 247 and name CB)	11.70	0.55	0.54
	assign	(segid 3A4 and resid 75 and name CB)	(segid 3A4 and resid 248 and name CA)	15.67	0.54	0.54
	assign	(segid 3A4 and resid 75 and name CB)	(segid 3A4 and resid 248 and name CB)	16.83	0.58	0.58
	assign	(segid 3A4 and resid 75 and name CB)	(segid 3A4 and resid 249 and name CA)	16.27	0.67	0.67
15	assign	(segid 3A4 and resid 75 and name CB)	(segid 3A4 and resid 250 and name CB)	13.58	0.59	0.59
	assign	(segid 3A4 and resid 75 and name CB)	(segid 3A4 and resid 251 and name CA)	12.08	0.60	0.61
	assign	(segid 3A4 and resid 75 and name CB)	(segid 3A4 and resid 251 and name CB)	14.96	0.41	0.42
	assign	(segid 3A4 and resid 75 and name CB)	(segid 3A4 and resid 252 and name CA)	15.13	0.37	0.37
	assign	(segid 3A4 and resid 75 and name CB)	(segid 3A4 and resid 252 and name CB)	18.39	0.46	0.47
20	assign	(segid 3A4 and resid 75 and name CB)	(segid 3A4 and resid 253 and name CA)	19.06	0.49	0.49
	assign	(segid 3A4 and resid 75 and name CB)	(segid 3A4 and resid 254 and name CA)	18.07	0.60	0.59
	assign	(segid 3A4 and resid 75 and name CB)	(segid 3A4 and resid 255 and name CA)	16.14	0.51	0.50
	assign	(segid 3A4 and resid 75 and name CB)	(segid 3A4 and resid 255 and name CB)	18.42	0.64	0.64
	assign	(segid 3A4 and resid 75 and name CB)	(segid 3A4 and resid 319 and name CB)	18.44	0.36	0.35
25	assign	(segid 3A4 and resid 75 and name CB)	(segid 3A4 and resid 322 and name CA)	14.76	0.48	0.49
	assign	(segid 3A4 and resid 75 and name CB)	(segid 3A4 and resid 323 and name CA)	13.40	0.73	0.73
	assign	(segid 3A4 and resid 75 and name CB)	(segid 3A4 and resid 323 and name CB)	13.49	0.86	0.86
	assign	(segid 3A4 and resid 75 and name CB)	(segid 3A4 and resid 324 and name CA)	14.47	0.94	0.94
	assign	(segid 3A4 and resid 75 and name CB)	(segid 3A4 and resid 324 and name CB)	14.19	0.92	0.92
30	assign	(segid 3A4 and resid 75 and name CB)	(segid 3A4 and resid 325 and name CA)	15.91	1.23	1.24
	assign	(segid 3A4 and resid 75 and name CB)	(segid 3A4 and resid 325 and name CB)	17.36	1.23	1.23
	assign	(segid 3A4 and resid 75 and name CB)	(segid 3A4 and resid 326 and name CA)	14.95	1.30	1.30
	assign	(segid 3A4 and resid 75 and name CB)	(segid 3A4 and resid 326 and name CB)	13.87	1.41	1.41
	assign	(segid 3A4 and resid 75 and name CB)	(segid 3A4 and resid 340 and name CA)	18.47	1.43	1.42
35	assign	(segid 3A4 and resid 75 and name CB)	(segid 3A4 and resid 342 and name CA)	18.34	0.86	0.86
	assign	(segid 3A4 and resid 75 and name CB)	(segid 3A4 and resid 343 and name CA)	18.38	0.88	0.87
	assign	(segid 3A4 and resid 75 and name CB)	(segid 3A4 and resid 343 and name CB)	17.92	1.02	1.02
	assign	(segid 3A4 and resid 75 and name CB)	(segid 3A4 and resid 344 and name CA)	18.86	0.57	0.56
	assign	(segid 3A4 and resid 75 and name CB)	(segid 3A4 and resid 345 and name CB)	17.56	0.91	0.91
40	assign	(segid 3A4 and resid 75 and name CB)	(segid 3A4 and resid 384 and name CA)	16.67	0.37	0.37
	assign	(segid 3A4 and resid 75 and name CB)	(segid 3A4 and resid 384 and name CB)	16.79	0.34	0.35
	assign	(segid 3A4 and resid 75 and name CB)	(segid 3A4 and resid 385 and name CA)	14.82	0.64	0.63
	assign	(segid 3A4 and resid 75 and name CB)	(segid 3A4 and resid 386 and name CA)	14.05	0.73	0.73
	assign	(segid 3A4 and resid 75 and name CB)	(segid 3A4 and resid 387 and name CA)	11.62	0.84	0.84
45	assign	(segid 3A4 and resid 75 and name CB)	(segid 3A4 and resid 388 and name CA)	8.22	1.00	0.99
	assign	(segid 3A4 and resid 75 and name CB)	(segid 3A4 and resid 388 and name CB)	7.36	1.20	1.19
	assign	(segid 3A4 and resid 75 and name CB)	(segid 3A4 and resid 389 and name CA)	7.88	0.51	0.50
	assign	(segid 3A4 and resid 75 and name CB)	(segid 3A4 and resid 389 and name CB)	7.84	0.45	

	assign	(segid 3A4 and resid 75 and name CB)	(segid 3A4 and resid 83 and name CA)	12.30	0.15	0.15
	assign	(segid 3A4 and resid 75 and name CB)	(segid 3A4 and resid 83 and name CB)	11.63	0.27	0.28
	assign	(segid 3A4 and resid 75 and name CB)	(segid 3A4 and resid 84 and name CA)	15.40	0.31	0.31
	assign	(segid 3A4 and resid 75 and name CB)	(segid 3A4 and resid 84 and name CB)	15.66	0.51	0.51
5	assign	(segid 3A4 and resid 75 and name CB)	(segid 3A4 and resid 85 and name CA)	16.89	0.37	0.38
	assign	(segid 3A4 and resid 75 and name CB)	(segid 3A4 and resid 85 and name CB)	16.68	0.51	0.52
	assign	(segid 3A4 and resid 75 and name CB)	(segid 3A4 and resid 86 and name CA)	16.31	0.14	0.14
	assign	(segid 3A4 and resid 75 and name CB)	(segid 3A4 and resid 86 and name CB)	15.25	0.33	0.32
	assign	(segid 3A4 and resid 75 and name CG)	(segid 3A4 and resid 388 and name C)	6.26	0.67	0.68
10	assign	(segid 3A4 and resid 75 and name CG)	(segid 3A4 and resid 388 and name O)	5.70	0.55	0.55
	assign	(segid 3A4 and resid 75 and name CG)	(segid 3A4 and resid 389 and name CA)	6.47	0.46	0.46
	assign	(segid 3A4 and resid 75 and name CG)	(segid 3A4 and resid 389 and name CB)	6.55	0.41	0.41
	assign	(segid 3A4 and resid 75 and name CG)	(segid 3A4 and resid 389 and name N)	6.63	0.64	0.63
	assign	(segid 3A4 and resid 75 and name CG)	(segid HEM and resid 1 and name CBD)	7.13	0.18	0.18
15	assign	(segid 3A4 and resid 75 and name CG)	(segid HEM and resid 1 and name CGD)	5.68	0.21	0.22
	assign	(segid 3A4 and resid 75 and name CG)	(segid HEM and resid 1 and name OLD)	5.07	0.25	0.25
	assign	(segid 3A4 and resid 75 and name CG)	(segid HEM and resid 1 and name O2D)	5.45	0.31	0.30
	assign	(segid 3A4 and resid 75 and name CG)	(segid 3A4 and resid 76 and name C)	5.61	0.21	0.22
	assign	(segid 3A4 and resid 75 and name CG)	(segid 3A4 and resid 76 and name CA)	4.55	0.24	0.24
20	assign	(segid 3A4 and resid 75 and name CG)	(segid 3A4 and resid 76 and name CB)	5.49	0.27	0.28
	assign	(segid 3A4 and resid 75 and name CG)	(segid 3A4 and resid 76 and name N)	3.52	0.26	0.27
	assign	(segid 3A4 and resid 75 and name CG)	(segid 3A4 and resid 76 and name O)	6.28	0.22	0.23
	assign	(segid 3A4 and resid 75 and name CG)	(segid 3A4 and resid 77 and name C)	7.32	0.16	0.16
	assign	(segid 3A4 and resid 75 and name CG)	(segid 3A4 and resid 77 and name CA)	7.33	0.21	0.21
25	assign	(segid 3A4 and resid 75 and name CG)	(segid 3A4 and resid 77 and name N)	6.10	0.23	0.23
	assign	(segid 3A4 and resid 75 and name CG)	(segid 3A4 and resid 78 and name C)	6.75	0.09	0.10
	assign	(segid 3A4 and resid 75 and name CG)	(segid 3A4 and resid 78 and name CA)	6.92	0.12	0.11
	assign	(segid 3A4 and resid 75 and name CG)	(segid 3A4 and resid 78 and name CB)	6.55	0.26	0.26
	assign	(segid 3A4 and resid 75 and name CG)	(segid 3A4 and resid 78 and name N)	6.54	0.07	0.07
30	assign	(segid 3A4 and resid 75 and name CG)	(segid 3A4 and resid 79 and name C)	7.28	0.14	0.13
	assign	(segid 3A4 and resid 75 and name CG)	(segid 3A4 and resid 79 and name CA)	5.99	0.10	0.10
	assign	(segid 3A4 and resid 75 and name CG)	(segid 3A4 and resid 79 and name CB)	4.95	0.13	0.12
	assign	(segid 3A4 and resid 75 and name CG)	(segid 3A4 and resid 79 and name CG)	5.74	0.14	0.14
	assign	(segid 3A4 and resid 75 and name CG)	(segid 3A4 and resid 79 and name N)	5.72	0.09	0.09
35	assign	(segid 3A4 and resid 75 and name CG)	(segid 3A4 and resid 80 and name N)	7.51	0.22	0.21
	assign	(segid 3A4 and resid 75 and name N)	(segid 3A4 and resid 75 and name C)	2.45	0.03	0.03
	assign	(segid 3A4 and resid 75 and name N)	(segid 3A4 and resid 75 and name CA)	1.46	0.01	0.02
	assign	(segid 3A4 and resid 75 and name N)	(segid 3A4 and resid 75 and name CB)	2.45	0.03	0.03
	assign	(segid 3A4 and resid 75 and name N)	(segid 3A4 and resid 75 and name CG)	3.80	0.02	0.03
40	assign	(segid 3A4 and resid 75 and name N)	(segid 3A4 and resid 75 and name O)	3.41	0.10	0.10
	assign	(segid 3A4 and resid 75 and name N)	(segid 3A4 and resid 76 and name C)	4.87	0.10	0.10
	assign	(segid 3A4 and resid 75 and name N)	(segid 3A4 and resid 76 and name CA)	4.31	0.08	0.09
	assign	(segid 3A4 and resid 75 and name N)	(segid 3A4 and resid 76 and name CB)	5.06	0.13	0.13
	assign	(segid 3A4 and resid 75 and name N)	(segid 3A4 and resid 76 and name N)	2.92	0.11	0.11
45	assign	(segid 3A4 and resid 75 and name N)	(segid 3A4 and resid 76 and name O)	5.98	0.13	0.12
	assign	(segid 3A4 and resid 75 and name N)	(segid 3A4 and resid 77 and name C)	5.82	0.25	0.25
	assign	(segid 3A4 and resid 75 and name N)	(segid 3A4 and resid 77 and name CA)	5.51	0.26	0.25
	assign	(segid 3A4 and resid 75 and name N)	(segid 3A4 and resid 77 and name CB)	5.61	0.38	0.37
	assign	(segid 3A4 and resid 75 and name N)	(segid 3A4 and resid 77 and name N)	4.48	0.19	0.19
50	assign	(segid 3A4 and resid 75 and name N)	(segid 3A4 and resid 77 and name O)	7.02	0.26	0.26
	assign	(segid 3A4 and resid 75 and name N)	(segid 3A4 and resid 78 and name C)	6.50	0.25	0.24
	assign	(segid 3A4 and resid 75 and name N)	(segid 3A4 and resid 78 and name CA)	5.83	0.24	0.23
	assign	(segid 3A4 and resid 75 and name N)	(segid 3A4 and resid 78 and name CB)	5.37	0.28	0.28
	assign	(segid 3A4 and resid 75 and name N)	(segid 3A4 and resid 78 and name N)	5.02	0.24	0.24
55	assign	(segid 3A4 and resid 75 and name N)	(segid 3A4 and resid 79 and name CA)	7.00	0.20	0.21
	assign	(segid 3A4 and resid 75 and name N)	(segid 3A4 and resid 79 and name CB)	6.61	0.16	0.16
	assign	(segid 3A4 and resid 75 and name N)	(segid 3A4 and resid 79 and name N)	5.98	0.21	0.21
	assign	(segid 3A4 and resid 75 and name O)	(segid HEM and resid 1 and name OLD)	6.51	0.45	0.46
	assign	(segid 3A4 and resid 75 and name O)	(segid 3A4 and resid 75 and name CB)	3.42	0.09	0.09
60	assign	(segid 3A4 and resid 75 and name O)	(segid 3A4 and resid 75 and name CG)	3.49	0.18	0.18
	assign	(segid 3A4 and resid 75 and name O)	(segid 3A4 and resid 76 and name C)	2.88	0.12	0.12
	assign	(segid 3A4 and resid 75 and name O)	(segid 3A4 and resid 76 and name CA)	2.78	0.03	0.03
	assign	(segid 3A4 and resid 75 and name O)	(segid 3A4 and resid 76 and name CB)	4.25	0.03	0.04
	assign	(segid 3A4 and resid 75 and name O)	(segid 3A4 and resid 76 and name N)	2.23	0.01	0.02
65	assign	(segid 3A4 and resid 75 and name O)	(segid 3A4 and resid 76 and name O)	3.47	0.12	0.13
	assign	(segid 3A4 and resid 75 and name O)	(segid 3A4 and resid 77 and name C)	3.87	0.26	0.26
	assign	(segid 3A4 and resid 75 and name O)	(segid 3A4 and resid 77 and name CA)	4.10	0.27	0.27
	assign	(segid 3A4 and resid 75 and name O)	(segid 3A4 and resid 77 and name CB)	5.07	0.30	0.29
	assign	(segid 3A4 and resid 75 and name O)	(segid 3A4 and resid 77 and name N)	3.17	0.24	0.24
70	assign	(segid 3A4 and resid 75 and name O)	(segid 3A4 and resid 77 and name O)	4.79	0.27	0.28
	assign	(segid 3A4 and resid 75 and name O)	(segid 3A4 and resid 78 and name C)	3.72	0.09	0.09
	assign	(segid 3A4 and resid 75 and name O)	(segid 3A4 and resid 78 and name CA)	3.73	0.15	0.14
	assign	(segid 3A4 and resid 75 and name O)	(segid 3A4 and resid 78 and name CB)	3.87	0.16	0.16
	assign	(segid 3A4 and resid 75 and name O)	(segid 3A4 and resid 78 and name N)	3.15	0.19	0.20
75	assign	(segid 3A4 and resid 75 and name O)	(segid 3A4 and resid 78 and name O)	4.89	0.09	0.09
	assign	(segid 3A4 and resid 75 and name O)	(segid 3A4 and resid 79 and name C)	4.77	0.10	0.11
	assign	(segid 3A4 and resid 75 and name O)	(segid 3A4 and resid 79 and name CA)	3.68	0.08	0.08
	assign	(segid 3A4 and resid 75 and name O)	(segid 3A4 and resid 79 and name CB)	3.34	0.15	0.15
	assign	(segid 3A4 and resid 75 and name O)	(segid 3A4 and resid 79 and name CG)	4.77	0.16	0.16
80	assign	(segid 3A4 and resid 75 and name O)	(segid 3A4 and resid 79 and name N)	2.82	0.06	0.06
	assign	(segid 3A4 and resid 75 and name O)	(segid 3A4 and resid 79 and name O)	5.93	0.11	0.12
	assign	(segid 3A4 and resid 75 and name O)	(segid 3A4 and resid 80 and name C)	6.99	0.15	0.16
	assign	(segid 3A4 and resid 75 and name O)	(segid 3A4 and resid 80 and name CA)	6.05	0.17	0.17

	assign (segid 3A4 and resid 75 and name O) (segid 3A4 and resid 80 and name N)	4.73	0.15	0.15
	assign (segid 3A4 and resid 75 and name O) (segid 3A4 and resid 81 and name N)	6.74	0.16	0.15
	assign (segid 3A4 and resid 76 and name C) (segid 3A4 and resid 76 and name CB)	2.50	0.04	0.04
	assign (segid 3A4 and resid 76 and name C) (segid 3A4 and resid 76 and name O)	1.24	0.01	0.01
	assign (segid 3A4 and resid 76 and name C) (segid 3A4 and resid 77 and name C)	3.06	0.04	0.04
5	assign (segid 3A4 and resid 76 and name C) (segid 3A4 and resid 77 and name CA)	2.42	0.01	0.01
	assign (segid 3A4 and resid 76 and name C) (segid 3A4 and resid 77 and name CB)	3.68	0.03	0.04
	assign (segid 3A4 and resid 76 and name C) (segid 3A4 and resid 77 and name N)	1.33	0.01	0.01
	assign (segid 3A4 and resid 76 and name C) (segid 3A4 and resid 77 and name O)	3.85	0.07	0.07
	assign (segid 3A4 and resid 76 and name C) (segid 3A4 and resid 78 and name C)	4.64	0.09	0.10
10	assign (segid 3A4 and resid 76 and name C) (segid 3A4 and resid 78 and name CA)	4.61	0.11	0.11
	assign (segid 3A4 and resid 76 and name C) (segid 3A4 and resid 78 and name CB)	5.49	0.15	0.14
	assign (segid 3A4 and resid 76 and name C) (segid 3A4 and resid 78 and name N)	3.42	0.11	0.12
	assign (segid 3A4 and resid 76 and name C) (segid 3A4 and resid 78 and name O)	5.65	0.12	0.12
	assign (segid 3A4 and resid 76 and name C) (segid 3A4 and resid 79 and name C)	4.83	0.03	0.04
15	assign (segid 3A4 and resid 76 and name C) (segid 3A4 and resid 79 and name CA)	4.59	0.07	0.07
	assign (segid 3A4 and resid 76 and name C) (segid 3A4 and resid 79 and name CB)	4.39	0.13	0.13
	assign (segid 3A4 and resid 76 and name C) (segid 3A4 and resid 79 and name CG)	5.56	0.16	0.16
	assign (segid 3A4 and resid 76 and name C) (segid 3A4 and resid 79 and name N)	3.91	0.07	0.08
	assign (segid 3A4 and resid 76 and name C) (segid 3A4 and resid 79 and name O)	6.04	0.05	0.04
20	assign (segid 3A4 and resid 76 and name C) (segid 3A4 and resid 80 and name C)	6.00	0.09	0.08
	assign (segid 3A4 and resid 76 and name C) (segid 3A4 and resid 80 and name CA)	4.83	0.12	0.13
	assign (segid 3A4 and resid 76 and name C) (segid 3A4 and resid 80 and name N)	4.02	0.06	0.07
	assign (segid 3A4 and resid 76 and name C) (segid 3A4 and resid 80 and name O)	7.10	0.11	0.11
	assign (segid 3A4 and resid 76 and name C) (segid 3A4 and resid 81 and name C)	7.32	0.10	0.11
25	assign (segid 3A4 and resid 76 and name C) (segid 3A4 and resid 81 and name CB)	7.45	0.16	0.16
	assign (segid 3A4 and resid 76 and name C) (segid 3A4 and resid 81 and name N)	5.99	0.09	0.09
	assign (segid 3A4 and resid 76 and name C) (segid 3A4 and resid 81 and name CA)	17.81	0.73	0.73
	assign (segid 3A4 and resid 76 and name CA) (segid 3A4 and resid 220 and name CB)	17.32	0.73	0.73
	assign (segid 3A4 and resid 76 and name CA) (segid 3A4 and resid 221 and name CA)	18.68	0.46	0.45
30	assign (segid 3A4 and resid 76 and name CA) (segid 3A4 and resid 223 and name CA)	17.16	0.68	0.67
	assign (segid 3A4 and resid 76 and name CA) (segid 3A4 and resid 223 and name CB)	16.62	0.81	0.81
	assign (segid 3A4 and resid 76 and name CA) (segid 3A4 and resid 224 and name CA)	14.92	0.46	0.45
	assign (segid 3A4 and resid 76 and name CA) (segid 3A4 and resid 224 and name CB)	14.71	0.39	0.39
35	assign (segid 3A4 and resid 76 and name CA) (segid 3A4 and resid 225 and name CA)	17.76	0.54	0.54
	assign (segid 3A4 and resid 76 and name CA) (segid 3A4 and resid 225 and name CB)	19.15	0.51	0.52
	assign (segid 3A4 and resid 76 and name CA) (segid 3A4 and resid 226 and name CA)	18.19	0.61	0.61
	assign (segid 3A4 and resid 76 and name CA) (segid 3A4 and resid 240 and name CA)	15.62	1.03	1.02
	assign (segid 3A4 and resid 76 and name CA) (segid 3A4 and resid 240 and name CB)	15.64	1.13	1.13
40	assign (segid 3A4 and resid 76 and name CA) (segid 3A4 and resid 241 and name CA)	18.03	0.77	0.76
	assign (segid 3A4 and resid 76 and name CA) (segid 3A4 and resid 242 and name CA)	17.20	0.81	0.81
	assign (segid 3A4 and resid 76 and name CA) (segid 3A4 and resid 242 and name CB)	17.42	0.92	0.92
	assign (segid 3A4 and resid 76 and name CA) (segid 3A4 and resid 243 and name CA)	13.54	0.74	0.75
	assign (segid 3A4 and resid 76 and name CA) (segid 3A4 and resid 243 and name CB)	12.49	0.85	0.85
45	assign (segid 3A4 and resid 76 and name CA) (segid 3A4 and resid 244 and name CA)	14.81	0.56	0.56
	assign (segid 3A4 and resid 76 and name CA) (segid 3A4 and resid 244 and name CB)	15.77	0.56	0.55
	assign (segid 3A4 and resid 76 and name CA) (segid 3A4 and resid 245 and name CA)	17.42	0.52	0.52
	assign (segid 3A4 and resid 76 and name CA) (segid 3A4 and resid 245 and name CB)	18.48	0.59	0.60
	assign (segid 3A4 and resid 76 and name CA) (segid 3A4 and resid 246 and name CA)	15.34	0.49	0.50
	assign (segid 3A4 and resid 76 and name CA) (segid 3A4 and resid 246 and name CB)	14.64	0.53	0.53
50	assign (segid 3A4 and resid 76 and name CA) (segid 3A4 and resid 247 and name CA)	13.22	0.37	0.36
	assign (segid 3A4 and resid 76 and name CA) (segid 3A4 and resid 247 and name CB)	12.41	0.35	0.36
	assign (segid 3A4 and resid 76 and name CA) (segid 3A4 and resid 248 and name CA)	16.61	0.41	0.40
	assign (segid 3A4 and resid 76 and name CA) (segid 3A4 and resid 248 and name CB)	17.63	0.43	0.42
	assign (segid 3A4 and resid 76 and name CA) (segid 3A4 and resid 249 and name CA)	18.09	0.44	0.45
55	assign (segid 3A4 and resid 76 and name CA) (segid 3A4 and resid 250 and name CA)	15.65	0.48	0.49
	assign (segid 3A4 and resid 76 and name CA) (segid 3A4 and resid 250 and name CB)	14.21	0.51	0.51
	assign (segid 3A4 and resid 76 and name CA) (segid 3A4 and resid 251 and name CA)	16.17	0.48	0.49
	assign (segid 3A4 and resid 76 and name CA) (segid 3A4 and resid 251 and name CB)	15.96	0.51	0.50
	assign (segid 3A4 and resid 76 and name CA) (segid 3A4 and resid 254 and name CA)	18.21	0.52	0.52
60	assign (segid 3A4 and resid 76 and name CA) (segid 3A4 and resid 322 and name CA)	18.57	0.64	0.64
	assign (segid 3A4 and resid 76 and name CA) (segid 3A4 and resid 323 and name CA)	17.13	0.89	0.89
	assign (segid 3A4 and resid 76 and name CA) (segid 3A4 and resid 323 and name CB)	17.02	0.90	0.89
	assign (segid 3A4 and resid 76 and name CA) (segid 3A4 and resid 324 and name CA)	18.23	1.22	1.22
	assign (segid 3A4 and resid 76 and name CA) (segid 3A4 and resid 324 and name CB)	18.06	1.19	1.19
65	assign (segid 3A4 and resid 76 and name CA) (segid 3A4 and resid 326 and name CA)	17.89	1.75	1.74
	assign (segid 3A4 and resid 76 and name CA) (segid 3A4 and resid 326 and name CB)	16.63	1.82	1.82
	assign (segid 3A4 and resid 76 and name CA) (segid 3A4 and resid 384 and name CA)	18.00	0.40	0.41
	assign (segid 3A4 and resid 76 and name CA) (segid 3A4 and resid 384 and name CB)	17.77	0.45	0.46
	assign (segid 3A4 and resid 76 and name CA) (segid 3A4 and resid 385 and name CA)	16.56	0.44	0.44
70	assign (segid 3A4 and resid 76 and name CA) (segid 3A4 and resid 386 and name CA)	15.28	0.43	0.43
	assign (segid 3A4 and resid 76 and name CA) (segid 3A4 and resid 387 and name CA)	12.49	0.51	0.51
	assign (segid 3A4 and resid 76 and name CA) (segid 3A4 and resid 388 and name CA)	8.78	0.54	0.55
	assign (segid 3A4 and resid 76 and name CA) (segid 3A4 and resid 388 and name CB)	7.99	0.53	0.53
	assign (segid 3A4 and resid 76 and name CA) (segid 3A4 and resid 389 and name CA)	9.63	0.36	0.36
75	assign (segid 3A4 and resid 76 and name CA) (segid 3A4 and resid 389 and name CB)	10.21	0.29	0.28
	assign (segid 3A4 and resid 76 and name CA) (segid 3A4 and resid 390 and name CA)	12.29	0.51	0.52
	assign (segid 3A4 and resid 76 and name CA) (segid 3A4 and resid 390 and name CB)	12.64	0.63	0.64
	assign (segid 3A4 and resid 76 and name CA) (segid 3A4 and resid 391 and name CA)	13.60	0.46	0.45
	assign (segid 3A4 and resid 76 and name CA) (segid 3A4 and resid 391 and name CB)	15.11	0.46	0.45
80	assign (segid 3A4 and resid 76 and name CA) (segid 3A4 and resid 392 and name CA)	12.14	0.47	0.46
	assign (segid 3A4 and resid 76 and name CA) (segid 3A4 and resid 392 and name CB)	11.22	0.41	0.41
	assign (segid 3A4 and resid 76 and name CA) (segid 3A4 and resid 393 and name CA)	15.70	0.42	0.43

	assign (segid 3A4 and resid 76 and name CA) (segid 3A4 and resid 394 and name CA)	17.51	0.53	0.53
	assign (segid 3A4 and resid 76 and name CA) (segid 3A4 and resid 394 and name CB)	17.06	0.55	0.55
	assign (segid 3A4 and resid 76 and name CA) (segid 3A4 and resid 76 and name C)	1.52	0.01	0.01
	assign (segid 3A4 and resid 76 and name CA) (segid 3A4 and resid 76 and name CB)	1.53	0.01	0.01
5	assign (segid 3A4 and resid 76 and name CA) (segid 3A4 and resid 76 and name O)	2.41	0.02	0.02
	assign (segid 3A4 and resid 76 and name CA) (segid 3A4 and resid 77 and name C)	4.44	0.04	0.04
	assign (segid 3A4 and resid 76 and name CA) (segid 3A4 and resid 77 and name CA)	3.79	0.01	0.01
	assign (segid 3A4 and resid 76 and name CA) (segid 3A4 and resid 77 and name CB)	4.82	0.05	0.06
	assign (segid 3A4 and resid 76 and name CA) (segid 3A4 and resid 77 and name N)	2.42	0.01	0.02
10	assign (segid 3A4 and resid 76 and name CA) (segid 3A4 and resid 77 and name O)	5.30	0.07	0.07
	assign (segid 3A4 and resid 76 and name CA) (segid 3A4 and resid 78 and name C)	5.56	0.12	0.12
	assign (segid 3A4 and resid 76 and name CA) (segid 3A4 and resid 78 and name CA)	5.59	0.12	0.13
	assign (segid 3A4 and resid 76 and name CA) (segid 3A4 and resid 78 and name CB)	6.20	0.18	0.17
	assign (segid 3A4 and resid 76 and name CA) (segid 3A4 and resid 78 and name N)	4.50	0.12	0.12
15	assign (segid 3A4 and resid 76 and name CA) (segid 3A4 and resid 78 and name O)	6.62	0.13	0.13
	assign (segid 3A4 and resid 76 and name CA) (segid 3A4 and resid 79 and name C)	5.58	0.13	0.14
	assign (segid 3A4 and resid 76 and name CA) (segid 3A4 and resid 79 and name CA)	5.10	0.15	0.15
	assign (segid 3A4 and resid 76 and name CA) (segid 3A4 and resid 79 and name CB)	4.45	0.20	0.19
	assign (segid 3A4 and resid 76 and name CA) (segid 3A4 and resid 79 and name CG)	5.49	0.24	0.24
20	assign (segid 3A4 and resid 76 and name CA) (segid 3A4 and resid 79 and name O)	4.60	0.12	0.12
	assign (segid 3A4 and resid 76 and name CA) (segid 3A4 and resid 80 and name C)	7.17	0.11	0.12
	assign (segid 3A4 and resid 76 and name CA) (segid 3A4 and resid 80 and name CA)	5.89	0.15	0.16
	assign (segid 3A4 and resid 76 and name CA) (segid 3A4 and resid 80 and name N)	4.98	0.13	0.13
25	assign (segid 3A4 and resid 76 and name CA) (segid 3A4 and resid 81 and name CA)	8.64	0.10	0.09
	assign (segid 3A4 and resid 76 and name CA) (segid 3A4 and resid 81 and name CB)	8.81	0.13	0.13
	assign (segid 3A4 and resid 76 and name CA) (segid 3A4 and resid 81 and name N)	7.27	0.09	0.09
	assign (segid 3A4 and resid 76 and name CA) (segid 3A4 and resid 82 and name CA)	10.10	0.23	0.23
	assign (segid 3A4 and resid 76 and name CA) (segid 3A4 and resid 82 and name CB)	10.01	0.51	0.50
30	assign (segid 3A4 and resid 76 and name CA) (segid 3A4 and resid 83 and name CA)	10.12	0.34	0.33
	assign (segid 3A4 and resid 76 and name CA) (segid 3A4 and resid 83 and name CB)	9.18	0.48	0.47
	assign (segid 3A4 and resid 76 and name CA) (segid 3A4 and resid 84 and name CA)	12.65	0.36	0.37
	assign (segid 3A4 and resid 76 and name CA) (segid 3A4 and resid 84 and name CB)	12.67	0.49	0.49
	assign (segid 3A4 and resid 76 and name CA) (segid 3A4 and resid 85 and name CA)	14.85	0.23	0.23
35	assign (segid 3A4 and resid 76 and name CA) (segid 3A4 and resid 85 and name CB)	14.82	0.34	0.34
	assign (segid 3A4 and resid 76 and name CA) (segid 3A4 and resid 86 and name CA)	14.89	0.28	0.29
	assign (segid 3A4 and resid 76 and name CA) (segid 3A4 and resid 86 and name CB)	14.14	0.47	0.48
	assign (segid 3A4 and resid 76 and name CB) (segid 3A4 and resid 223 and name CA)	18.22	0.69	0.69
	assign (segid 3A4 and resid 76 and name CB) (segid 3A4 and resid 223 and name CB)	17.69	0.83	0.83
40	assign (segid 3A4 and resid 76 and name CB) (segid 3A4 and resid 224 and name CA)	16.06	0.48	0.48
	assign (segid 3A4 and resid 76 and name CB) (segid 3A4 and resid 224 and name CB)	15.94	0.42	0.41
	assign (segid 3A4 and resid 76 and name CB) (segid 3A4 and resid 225 and name CA)	18.82	0.59	0.59
	assign (segid 3A4 and resid 76 and name CB) (segid 3A4 and resid 240 and name CA)	16.53	1.25	1.24
	assign (segid 3A4 and resid 76 and name CB) (segid 3A4 and resid 240 and name CB)	16.50	1.37	1.38
45	assign (segid 3A4 and resid 76 and name CB) (segid 3A4 and resid 243 and name CA)	14.73	0.89	0.90
	assign (segid 3A4 and resid 76 and name CB) (segid 3A4 and resid 243 and name CB)	13.62	1.01	1.01
	assign (segid 3A4 and resid 76 and name CB) (segid 3A4 and resid 244 and name CA)	16.09	0.65	0.66
	assign (segid 3A4 and resid 76 and name CB) (segid 3A4 and resid 244 and name CB)	17.01	0.66	0.66
	assign (segid 3A4 and resid 76 and name CB) (segid 3A4 and resid 245 and name CA)	18.77	0.61	0.61
50	assign (segid 3A4 and resid 76 and name CB) (segid 3A4 and resid 246 and name CA)	16.72	0.58	0.58
	assign (segid 3A4 and resid 76 and name CB) (segid 3A4 and resid 246 and name CB)	15.97	0.64	0.64
	assign (segid 3A4 and resid 76 and name CB) (segid 3A4 and resid 247 and name CA)	14.68	0.40	0.39
	assign (segid 3A4 and resid 76 and name CB) (segid 3A4 and resid 247 and name CB)	13.86	0.38	0.39
	assign (segid 3A4 and resid 76 and name CB) (segid 3A4 and resid 248 and name CA)	18.06	0.43	0.43
55	assign (segid 3A4 and resid 76 and name CB) (segid 3A4 and resid 250 and name CA)	17.11	0.50	0.50
	assign (segid 3A4 and resid 76 and name CB) (segid 3A4 and resid 250 and name CB)	15.66	0.53	0.53
	assign (segid 3A4 and resid 76 and name CB) (segid 3A4 and resid 251 and name CA)	17.63	0.54	0.54
	assign (segid 3A4 and resid 76 and name CB) (segid 3A4 and resid 251 and name CB)	17.41	0.56	0.57
	assign (segid 3A4 and resid 76 and name CB) (segid 3A4 and resid 323 and name CA)	17.55	0.91	0.92
60	assign (segid 3A4 and resid 76 and name CB) (segid 3A4 and resid 323 and name CB)	17.36	0.92	0.92
	assign (segid 3A4 and resid 76 and name CB) (segid 3A4 and resid 324 and name CA)	18.46	1.31	1.31
	assign (segid 3A4 and resid 76 and name CB) (segid 3A4 and resid 324 and name CB)	18.32	1.29	1.30
	assign (segid 3A4 and resid 76 and name CB) (segid 3A4 and resid 326 and name CA)	17.64	1.92	1.92
	assign (segid 3A4 and resid 76 and name CB) (segid 3A4 and resid 326 and name CB)	16.34	1.97	1.97
65	assign (segid 3A4 and resid 76 and name CB) (segid 3A4 and resid 384 and name CA)	18.58	0.72	0.71
	assign (segid 3A4 and resid 76 and name CB) (segid 3A4 and resid 385 and name CA)	17.21	0.64	0.65
	assign (segid 3A4 and resid 76 and name CB) (segid 3A4 and resid 386 and name CA)	15.64	0.69	0.69
	assign (segid 3A4 and resid 76 and name CB) (segid 3A4 and resid 387 and name CA)	12.64	0.78	0.78
	assign (segid 3A4 and resid 76 and name CB) (segid 3A4 and resid 388 and name CA)	9.01	0.79	0.79
70	assign (segid 3A4 and resid 76 and name CB) (segid 3A4 and resid 388 and name CB)	8.10	0.73	0.72
	assign (segid 3A4 and resid 76 and name CB) (segid 3A4 and resid 389 and name CA)	10.35	0.53	0.52
	assign (segid 3A4 and resid 76 and name CB) (segid 3A4 and resid 389 and name CB)	10.93	0.42	0.42
	assign (segid 3A4 and resid 76 and name CB) (segid 3A4 and resid 390 and name CA)	13.00	0.74	0.74
	assign (segid 3A4 and resid 76 and name CB) (segid 3A4 and resid 390 and name CB)	13.23	0.89	0.89
75	assign (segid 3A4 and resid 76 and name CB) (segid 3A4 and resid 391 and name CA)	14.59	0.68	0.68
	assign (segid 3A4 and resid 76 and name CB) (segid 3A4 and resid 391 and name CB)	16.11	0.68	0.68
	assign (segid 3A4 and resid 76 and name CB) (segid 3A4 and resid 392 and name CA)	13.24	0.69	0.68
	assign (segid 3A4 and resid 76 and name CB) (segid 3A4 and resid 392 and name CB)	12.41	0.60	0.60
	assign (segid 3A4 and resid 76 and name CB) (segid 3A4 and resid 393 and name CA)	16.85	0.65	0.65
80	assign (segid 3A4 and resid 76 and name CB) (segid 3A4 and resid 394 and name CA)	18.47	0.80	0.79
	assign (segid 3A4 and resid 76 and name CB) (segid 3A4 and resid 394 and name CB)	17.93	0.83	0.83
	assign (segid 3A4 and resid 76 and name CB) (segid 3A4 and resid 77 and name C)	5.46	0.07	0.06
	assign (segid 3A4 and resid 76 and name CB) (segid 3A4 and resid 77 and name CA)	4.47	0.08	0.08

	assign (segid 3A4 and resid 76 and name CB) (segid 3A4 and resid 77 and name CB)	5.29	0.14	0.13
	assign (segid 3A4 and resid 76 and name CB) (segid 3A4 and resid 77 and name N)	3.17	0.08	0.07
	assign (segid 3A4 and resid 76 and name CB) (segid 3A4 and resid 77 and name O)	6.28	0.10	0.10
	assign (segid 3A4 and resid 76 and name CB) (segid 3A4 and resid 78 and name C)	6.97	0.12	0.13
5	assign (segid 3A4 and resid 76 and name CB) (segid 3A4 and resid 78 and name CA)	6.94	0.11	0.11
	assign (segid 3A4 and resid 76 and name CB) (segid 3A4 and resid 78 and name CB)	7.58	0.17	0.17
	assign (segid 3A4 and resid 76 and name CB) (segid 3A4 and resid 78 and name N)	5.72	0.10	0.10
	assign (segid 3A4 and resid 76 and name CB) (segid 3A4 and resid 79 and name C)	6.80	0.22	0.21
	assign (segid 3A4 and resid 76 and name CB) (segid 3A4 and resid 79 and name CA)	6.48	0.20	0.21
10	assign (segid 3A4 and resid 76 and name CB) (segid 3A4 and resid 79 and name CB)	5.77	0.25	0.26
	assign (segid 3A4 and resid 76 and name CB) (segid 3A4 and resid 79 and name CG)	6.63	0.35	0.35
	assign (segid 3A4 and resid 76 and name CB) (segid 3A4 and resid 79 and name N)	6.06	0.14	0.15
	assign (segid 3A4 and resid 76 and name CB) (segid 3A4 and resid 80 and name CA)	6.71	0.21	0.21
	assign (segid 3A4 and resid 76 and name CB) (segid 3A4 and resid 80 and name N)	6.04	0.19	0.19
15	assign (segid 3A4 and resid 76 and name CB) (segid 3A4 and resid 81 and name CA)	9.64	0.14	0.15
	assign (segid 3A4 and resid 76 and name CB) (segid 3A4 and resid 81 and name CB)	9.87	0.20	0.19
	assign (segid 3A4 and resid 76 and name CB) (segid 3A4 and resid 82 and name CA)	11.33	0.20	0.21
	assign (segid 3A4 and resid 76 and name CB) (segid 3A4 and resid 82 and name CB)	11.33	0.45	0.45
	assign (segid 3A4 and resid 76 and name CB) (segid 3A4 and resid 83 and name CA)	11.09	0.49	0.50
20	assign (segid 3A4 and resid 76 and name CB) (segid 3A4 and resid 83 and name CB)	10.04	0.65	0.64
	assign (segid 3A4 and resid 76 and name CB) (segid 3A4 and resid 84 and name CA)	13.44	0.47	0.47
	assign (segid 3A4 and resid 76 and name CB) (segid 3A4 and resid 84 and name CB)	13.39	0.52	0.52
	assign (segid 3A4 and resid 76 and name CB) (segid 3A4 and resid 85 and name CA)	15.85	0.25	0.25
	assign (segid 3A4 and resid 76 and name CB) (segid 3A4 and resid 85 and name CB)	15.89	0.28	0.28
25	assign (segid 3A4 and resid 76 and name CB) (segid 3A4 and resid 86 and name CA)	15.95	0.54	0.53
	assign (segid 3A4 and resid 76 and name CB) (segid 3A4 and resid 86 and name CB)	15.26	0.67	0.67
	assign (segid 3A4 and resid 76 and name N) (segid 3A4 and resid 76 and name C)	2.50	0.02	0.01
	assign (segid 3A4 and resid 76 and name N) (segid 3A4 and resid 76 and name CA)	1.46	0.01	0.01
	assign (segid 3A4 and resid 76 and name N) (segid 3A4 and resid 76 and name CB)	2.47	0.02	0.01
30	assign (segid 3A4 and resid 76 and name N) (segid 3A4 and resid 76 and name O)	3.55	0.04	0.04
	assign (segid 3A4 and resid 76 and name N) (segid 3A4 and resid 77 and name C)	4.77	0.04	0.04
	assign (segid 3A4 and resid 76 and name N) (segid 3A4 and resid 77 and name CA)	4.24	0.07	0.08
	assign (segid 3A4 and resid 76 and name N) (segid 3A4 and resid 77 and name CB)	5.01	0.15	0.14
	assign (segid 3A4 and resid 76 and name N) (segid 3A4 and resid 77 and name N)	2.84	0.07	0.08
35	assign (segid 3A4 and resid 76 and name N) (segid 3A4 and resid 77 and name O)	5.81	0.07	0.08
	assign (segid 3A4 and resid 76 and name N) (segid 3A4 and resid 78 and name C)	5.65	0.02	0.02
	assign (segid 3A4 and resid 76 and name N) (segid 3A4 and resid 78 and name CA)	5.48	0.08	0.09
	assign (segid 3A4 and resid 76 and name N) (segid 3A4 and resid 78 and name CB)	5.73	0.19	0.19
	assign (segid 3A4 and resid 76 and name N) (segid 3A4 and resid 78 and name N)	4.46	0.09	0.08
40	assign (segid 3A4 and resid 76 and name N) (segid 3A4 and resid 78 and name O)	6.81	0.02	0.02
	assign (segid 3A4 and resid 76 and name N) (segid 3A4 and resid 79 and name C)	6.25	0.09	0.08
	assign (segid 3A4 and resid 76 and name N) (segid 3A4 and resid 79 and name CA)	5.44	0.10	0.10
	assign (segid 3A4 and resid 76 and name N) (segid 3A4 and resid 79 and name CB)	4.77	0.16	0.16
	assign (segid 3A4 and resid 76 and name N) (segid 3A4 and resid 79 and name CG)	5.94	0.19	0.19
45	assign (segid 3A4 and resid 76 and name N) (segid 3A4 and resid 79 and name N)	4.75	0.05	0.05
	assign (segid 3A4 and resid 76 and name N) (segid 3A4 and resid 79 and name O)	7.45	0.10	0.11
	assign (segid 3A4 and resid 76 and name N) (segid 3A4 and resid 80 and name CA)	6.95	0.15	0.14
	assign (segid 3A4 and resid 76 and name N) (segid 3A4 and resid 80 and name N)	5.86	0.11	0.10
	assign (segid 3A4 and resid 76 and name O) (segid 3A4 and resid 76 and name CB)	3.27	0.07	0.07
50	assign (segid 3A4 and resid 76 and name O) (segid 3A4 and resid 77 and name C)	3.06	0.07	0.07
	assign (segid 3A4 and resid 76 and name O) (segid 3A4 and resid 77 and name CA)	2.76	0.04	0.03
	assign (segid 3A4 and resid 76 and name O) (segid 3A4 and resid 77 and name CB)	4.22	0.04	0.03
	assign (segid 3A4 and resid 76 and name O) (segid 3A4 and resid 77 and name N)	2.26	0.02	0.01
	assign (segid 3A4 and resid 76 and name O) (segid 3A4 and resid 77 and name O)	3.45	0.11	0.12
55	assign (segid 3A4 and resid 76 and name O) (segid 3A4 and resid 78 and name C)	4.34	0.13	0.14
	assign (segid 3A4 and resid 76 and name O) (segid 3A4 and resid 78 and name CA)	4.62	0.14	0.14
	assign (segid 3A4 and resid 76 and name O) (segid 3A4 and resid 78 and name CB)	5.73	0.16	0.16
	assign (segid 3A4 and resid 76 and name O) (segid 3A4 and resid 78 and name N)	3.65	0.13	0.13
	assign (segid 3A4 and resid 76 and name O) (segid 3A4 and resid 78 and name O)	5.17	0.19	0.18
60	assign (segid 3A4 and resid 76 and name O) (segid 3A4 and resid 79 and name C)	3.94	0.05	0.04
	assign (segid 3A4 and resid 76 and name O) (segid 3A4 and resid 79 and name CA)	4.03	0.04	0.03
	assign (segid 3A4 and resid 76 and name O) (segid 3A4 and resid 79 and name CB)	3.96	0.10	0.10
	assign (segid 3A4 and resid 76 and name O) (segid 3A4 and resid 79 and name CG)	4.99	0.14	0.13
	assign (segid 3A4 and resid 76 and name O) (segid 3A4 and resid 79 and name N)	3.61	0.05	0.06
65	assign (segid 3A4 and resid 76 and name O) (segid 3A4 and resid 79 and name O)	5.08	0.07	0.06
	assign (segid 3A4 and resid 76 and name O) (segid 3A4 and resid 80 and name C)	4.88	0.10	0.10
	assign (segid 3A4 and resid 76 and name O) (segid 3A4 and resid 80 and name CA)	3.65	0.14	0.13
	assign (segid 3A4 and resid 76 and name O) (segid 3A4 and resid 80 and name N)	2.96	0.06	0.07
	assign (segid 3A4 and resid 76 and name O) (segid 3A4 and resid 80 and name O)	5.94	0.13	0.14
70	assign (segid 3A4 and resid 76 and name O) (segid 3A4 and resid 81 and name C)	7.35	0.11	0.12
	assign (segid 3A4 and resid 76 and name O) (segid 3A4 and resid 81 and name CA)	6.42	0.11	0.12
	assign (segid 3A4 and resid 76 and name O) (segid 3A4 and resid 81 and name CB)	6.76	0.16	0.15
	assign (segid 3A4 and resid 76 and name O) (segid 3A4 and resid 81 and name N)	5.03	0.11	0.11
	assign (segid 3A4 and resid 76 and name O) (segid 3A4 and resid 82 and name N)	7.13	0.16	0.17
75	assign (segid 3A4 and resid 76 and name O) (segid 3A4 and resid 83 and name CB)	7.48	0.36	0.36
	assign (segid 3A4 and resid 76 and name O) (segid 3A4 and resid 83 and name N)	7.77	0.08	0.08
	assign (segid 3A4 and resid 77 and name C) (segid 3A4 and resid 77 and name CB)	2.52	0.03	0.02
	assign (segid 3A4 and resid 77 and name C) (segid 3A4 and resid 77 and name O)	1.24	0.01	0.01
	assign (segid 3A4 and resid 77 and name C) (segid 3A4 and resid 78 and name C)	3.06	0.05	0.06
80	assign (segid 3A4 and resid 77 and name C) (segid 3A4 and resid 78 and name CA)	2.44	0.02	0.01
	assign (segid 3A4 and resid 77 and name C) (segid 3A4 and resid 78 and name CB)	3.70	0.03	0.03
	assign (segid 3A4 and resid 77 and name C) (segid 3A4 and resid 78 and name N)	1.33	0.01	0.01
	assign (segid 3A4 and resid 77 and name C) (segid 3A4 and resid 78 and name O)	3.88	0.12	0.12

assign (segid 3A4 and resid 77 and name C) (segid 3A4 and resid 79 and name C) 4.61 0.15 0.16
 assign (segid 3A4 and resid 77 and name C) (segid 3A4 and resid 79 and name CA) 4.52 0.11 0.12
 assign (segid 3A4 and resid 77 and name C) (segid 3A4 and resid 79 and name CB) 5.27 0.12 0.12
 assign (segid 3A4 and resid 77 and name C) (segid 3A4 and resid 79 and name CG) 6.62 0.12 0.12
 5 assign (segid 3A4 and resid 77 and name C) (segid 3A4 and resid 79 and name N) 3.33 0.12 0.12
 assign (segid 3A4 and resid 77 and name C) (segid 3A4 and resid 79 and name O) 5.66 0.18 0.18
 assign (segid 3A4 and resid 77 and name C) (segid 3A4 and resid 80 and name C) 5.02 0.20 0.20
 assign (segid 3A4 and resid 77 and name C) (segid 3A4 and resid 80 and name CA) 4.61 0.21 0.21
 assign (segid 3A4 and resid 77 and name C) (segid 3A4 and resid 80 and name N) 3.90 0.16 0.17
 10 assign (segid 3A4 and resid 77 and name C) (segid 3A4 and resid 80 and name O) 6.21 0.17 0.18
 assign (segid 3A4 and resid 77 and name C) (segid 3A4 and resid 81 and name C) 6.47 0.37 0.37
 assign (segid 3A4 and resid 77 and name C) (segid 3A4 and resid 81 and name CA) 5.34 0.27 0.27
 assign (segid 3A4 and resid 77 and name C) (segid 3A4 and resid 81 and name CB) 4.98 0.31 0.32
 assign (segid 3A4 and resid 77 and name C) (segid 3A4 and resid 81 and name N) 4.39 0.27 0.26
 15 assign (segid 3A4 and resid 77 and name C) (segid 3A4 and resid 82 and name N) 6.39 0.49 0.50
 assign (segid 3A4 and resid 77 and name CA) (segid 3A4 and resid 202 and name CB) 18.75 0.54 0.54
 assign (segid 3A4 and resid 77 and name CA) (segid 3A4 and resid 220 and name CA) 16.04 0.81 0.80
 assign (segid 3A4 and resid 77 and name CA) (segid 3A4 and resid 220 and name CB) 15.80 0.79 0.79
 assign (segid 3A4 and resid 77 and name CA) (segid 3A4 and resid 221 and name CA) 16.46 0.68 0.68
 20 assign (segid 3A4 and resid 77 and name CA) (segid 3A4 and resid 221 and name CB) 17.70 0.68 0.68
 assign (segid 3A4 and resid 77 and name CA) (segid 3A4 and resid 222 and name CA) 17.47 0.67 0.67
 assign (segid 3A4 and resid 77 and name CA) (segid 3A4 and resid 222 and name CB) 18.65 0.67 0.68
 assign (segid 3A4 and resid 77 and name CA) (segid 3A4 and resid 223 and name CA) 14.57 0.75 0.75
 assign (segid 3A4 and resid 77 and name CA) (segid 3A4 and resid 223 and name CB) 14.28 0.84 0.84
 25 assign (segid 3A4 and resid 77 and name CA) (segid 3A4 and resid 224 and name CA) 12.18 0.65 0.65
 assign (segid 3A4 and resid 77 and name CA) (segid 3A4 and resid 224 and name CB) 12.17 0.61 0.62
 assign (segid 3A4 and resid 77 and name CA) (segid 3A4 and resid 225 and name CA) 14.67 0.73 0.73
 assign (segid 3A4 and resid 77 and name CA) (segid 3A4 and resid 225 and name CB) 16.12 0.72 0.72
 assign (segid 3A4 and resid 77 and name CA) (segid 3A4 and resid 226 and name CA) 14.89 0.80 0.81
 30 assign (segid 3A4 and resid 77 and name CA) (segid 3A4 and resid 240 and name CA) 12.58 1.09 1.10
 assign (segid 3A4 and resid 77 and name CA) (segid 3A4 and resid 240 and name CB) 12.78 1.17 1.17
 assign (segid 3A4 and resid 77 and name CA) (segid 3A4 and resid 241 and name CA) 15.26 0.88 0.88
 assign (segid 3A4 and resid 77 and name CA) (segid 3A4 and resid 241 and name CB) 16.70 0.92 0.91
 assign (segid 3A4 and resid 77 and name CA) (segid 3A4 and resid 242 and name CA) 15.04 0.87 0.88
 35 assign (segid 3A4 and resid 77 and name CA) (segid 3A4 and resid 242 and name CB) 15.35 0.93 0.93
 assign (segid 3A4 and resid 77 and name CA) (segid 3A4 and resid 243 and name CA) 11.49 0.78 0.78
 assign (segid 3A4 and resid 77 and name CA) (segid 3A4 and resid 243 and name CB) 10.23 0.85 0.85
 assign (segid 3A4 and resid 77 and name CA) (segid 3A4 and resid 244 and name CA) 12.51 0.73 0.72
 assign (segid 3A4 and resid 77 and name CA) (segid 3A4 and resid 244 and name CB) 13.23 0.73 0.73
 40 assign (segid 3A4 and resid 77 and name CA) (segid 3A4 and resid 245 and name CA) 15.62 0.67 0.67
 assign (segid 3A4 and resid 77 and name CA) (segid 3A4 and resid 245 and name CB) 16.64 0.72 0.73
 assign (segid 3A4 and resid 77 and name CA) (segid 3A4 and resid 246 and name CA) 14.23 0.56 0.57
 assign (segid 3A4 and resid 77 and name CA) (segid 3A4 and resid 246 and name CB) 13.60 0.55 0.54
 assign (segid 3A4 and resid 77 and name CA) (segid 3A4 and resid 247 and name CA) 12.16 0.45 0.46
 45 assign (segid 3A4 and resid 77 and name CA) (segid 3A4 and resid 247 and name CB) 11.08 0.45 0.45
 assign (segid 3A4 and resid 77 and name CA) (segid 3A4 and resid 248 and name CA) 15.41 0.48 0.47
 assign (segid 3A4 and resid 77 and name CA) (segid 3A4 and resid 248 and name CB) 16.17 0.51 0.52
 assign (segid 3A4 and resid 77 and name CA) (segid 3A4 and resid 249 and name CA) 17.43 0.51 0.51
 50 assign (segid 3A4 and resid 77 and name CA) (segid 3A4 and resid 250 and name CA) 15.66 0.46 0.45
 assign (segid 3A4 and resid 77 and name CA) (segid 3A4 and resid 250 and name CB) 14.29 0.48 0.49
 assign (segid 3A4 and resid 77 and name CA) (segid 3A4 and resid 251 and name CA) 16.04 0.41 0.42
 assign (segid 3A4 and resid 77 and name CA) (segid 3A4 and resid 251 and name CB) 15.55 0.43 0.43
 assign (segid 3A4 and resid 77 and name CA) (segid 3A4 and resid 254 and name CA) 19.04 0.34 0.34
 55 assign (segid 3A4 and resid 77 and name CA) (segid 3A4 and resid 386 and name CA) 18.57 0.25 0.24
 assign (segid 3A4 and resid 77 and name CA) (segid 3A4 and resid 387 and name CA) 15.98 0.33 0.33
 assign (segid 3A4 and resid 77 and name CA) (segid 3A4 and resid 388 and name CA) 12.25 0.35 0.35
 assign (segid 3A4 and resid 77 and name CA) (segid 3A4 and resid 388 and name CB) 11.55 0.39 0.40
 assign (segid 3A4 and resid 77 and name CA) (segid 3A4 and resid 389 and name CA) 12.70 0.28 0.27
 60 assign (segid 3A4 and resid 77 and name CA) (segid 3A4 and resid 389 and name CB) 13.27 0.25 0.25
 assign (segid 3A4 and resid 77 and name CA) (segid 3A4 and resid 390 and name CA) 15.12 0.36 0.37
 assign (segid 3A4 and resid 77 and name CA) (segid 3A4 and resid 390 and name CB) 15.51 0.47 0.47
 assign (segid 3A4 and resid 77 and name CA) (segid 3A4 and resid 391 and name CA) 15.72 0.30 0.29
 assign (segid 3A4 and resid 77 and name CA) (segid 3A4 and resid 391 and name CB) 17.17 0.30 0.30
 65 assign (segid 3A4 and resid 77 and name CA) (segid 3A4 and resid 392 and name CA) 13.57 0.27 0.27
 assign (segid 3A4 and resid 77 and name CA) (segid 3A4 and resid 392 and name CB) 12.40 0.28 0.28
 assign (segid 3A4 and resid 77 and name CA) (segid 3A4 and resid 393 and name CA) 16.75 0.33 0.32
 assign (segid 3A4 and resid 77 and name CA) (segid 3A4 and resid 394 and name CA) 19.10 0.35 0.35
 assign (segid 3A4 and resid 77 and name CA) (segid 3A4 and resid 394 and name CB) 18.88 0.37 0.37
 70 assign (segid 3A4 and resid 77 and name C) 1.52 0.00 0.01
 assign (segid 3A4 and resid 77 and name CB) 1.53 0.01 0.00
 assign (segid 3A4 and resid 77 and name O) 2.40 0.02 0.01
 assign (segid 3A4 and resid 77 and name C) 4.44 0.05 0.04
 assign (segid 3A4 and resid 77 and name CA) 3.81 0.01 0.02
 75 assign (segid 3A4 and resid 77 and name CB) 4.87 0.02 0.02
 assign (segid 3A4 and resid 77 and name N) 2.43 0.01 0.02
 assign (segid 3A4 and resid 77 and name O) 5.33 0.12 0.11
 assign (segid 3A4 and resid 77 and name C) 5.55 0.14 0.14
 assign (segid 3A4 and resid 77 and name CA) 5.49 0.10 0.09
 80 assign (segid 3A4 and resid 77 and name CB) 5.90 0.12 0.12
 assign (segid 3A4 and resid 77 and name CG) 7.21 0.12 0.12
 assign (segid 3A4 and resid 77 and name N) 4.41 0.11 0.10
 assign (segid 3A4 and resid 77 and name O) 6.66 0.16 0.16
 assign (segid 3A4 and resid 77 and name CA) (segid 3A4 and resid 80 and name C) 5.85 0.22 0.22

	assign (segid 3A4 and resid 77 and name CA) (segid 3A4 and resid 80 and name CA)	5.18	0.23	0.23
	assign (segid 3A4 and resid 77 and name CA) (segid 3A4 and resid 80 and name N)	4.63	0.17	0.17
	assign (segid 3A4 and resid 77 and name CA) (segid 3A4 and resid 80 and name O)	7.00	0.19	0.19
	assign (segid 3A4 and resid 77 and name CA) (segid 3A4 and resid 81 and name CA)	6.48	0.31	0.31
5	assign (segid 3A4 and resid 77 and name CA) (segid 3A4 and resid 81 and name CB)	6.24	0.39	0.38
	assign (segid 3A4 and resid 77 and name CA) (segid 3A4 and resid 81 and name N)	5.43	0.30	0.30
	assign (segid 3A4 and resid 77 and name CA) (segid 3A4 and resid 82 and name CA)	9.03	0.50	0.49
	assign (segid 3A4 and resid 77 and name CA) (segid 3A4 and resid 82 and name CB)	9.20	0.68	0.68
	assign (segid 3A4 and resid 77 and name CA) (segid 3A4 and resid 83 and name CA)	10.04	0.18	0.17
10	assign (segid 3A4 and resid 77 and name CA) (segid 3A4 and resid 83 and name CB)	9.41	0.21	0.22
	assign (segid 3A4 and resid 77 and name CA) (segid 3A4 and resid 84 and name CA)	11.83	0.73	0.73
	assign (segid 3A4 and resid 77 and name CA) (segid 3A4 and resid 84 and name CB)	11.51	0.93	0.92
	assign (segid 3A4 and resid 77 and name CA) (segid 3A4 and resid 85 and name CA)	13.80	0.83	0.84
	assign (segid 3A4 and resid 77 and name CA) (segid 3A4 and resid 85 and name CB)	13.53	0.95	0.96
15	assign (segid 3A4 and resid 77 and name CA) (segid 3A4 and resid 86 and name CA)	14.72	0.49	0.49
	assign (segid 3A4 and resid 77 and name CA) (segid 3A4 and resid 86 and name CB)	14.15	0.49	0.50
	assign (segid 3A4 and resid 77 and name CB) (segid 3A4 and resid 202 and name CB)	18.60	0.74	0.74
	assign (segid 3A4 and resid 77 and name CB) (segid 3A4 and resid 220 and name CA)	16.70	0.93	0.92
	assign (segid 3A4 and resid 77 and name CB) (segid 3A4 and resid 220 and name CB)	16.52	0.92	0.93
20	assign (segid 3A4 and resid 77 and name CB) (segid 3A4 and resid 221 and name CA)	16.82	0.87	0.88
	assign (segid 3A4 and resid 77 and name CB) (segid 3A4 and resid 221 and name CB)	18.02	0.89	0.88
	assign (segid 3A4 and resid 77 and name CB) (segid 3A4 and resid 222 and name CA)	17.75	0.82	0.81
	assign (segid 3A4 and resid 77 and name CB) (segid 3A4 and resid 223 and name CA)	14.99	0.83	0.83
	assign (segid 3A4 and resid 77 and name CB) (segid 3A4 and resid 223 and name CB)	14.83	0.89	0.89
25	assign (segid 3A4 and resid 77 and name CB) (segid 3A4 and resid 224 and name CA)	12.41	0.82	0.82
	assign (segid 3A4 and resid 77 and name CB) (segid 3A4 and resid 224 and name CB)	12.43	0.80	0.81
	assign (segid 3A4 and resid 77 and name CB) (segid 3A4 and resid 225 and name CA)	14.58	0.89	0.89
	assign (segid 3A4 and resid 77 and name CB) (segid 3A4 and resid 225 and name CB)	16.05	0.89	0.89
	assign (segid 3A4 and resid 77 and name CB) (segid 3A4 and resid 226 and name CA)	14.80	0.94	0.94
30	assign (segid 3A4 and resid 77 and name CB) (segid 3A4 and resid 240 and name CA)	11.76	1.27	1.27
	assign (segid 3A4 and resid 77 and name CB) (segid 3A4 and resid 240 and name CB)	11.86	1.36	1.36
	assign (segid 3A4 and resid 77 and name CB) (segid 3A4 and resid 241 and name CA)	14.67	1.10	1.09
	assign (segid 3A4 and resid 77 and name CB) (segid 3A4 and resid 241 and name CB)	16.07	1.13	1.13
	assign (segid 3A4 and resid 77 and name CB) (segid 3A4 and resid 242 and name CA)	14.48	1.07	1.08
35	assign (segid 3A4 and resid 77 and name CB) (segid 3A4 and resid 242 and name CB)	14.70	1.12	1.12
	assign (segid 3A4 and resid 77 and name CB) (segid 3A4 and resid 243 and name CA)	11.08	0.95	0.95
	assign (segid 3A4 and resid 77 and name CB) (segid 3A4 and resid 243 and name CB)	9.73	1.01	1.01
	assign (segid 3A4 and resid 77 and name CB) (segid 3A4 and resid 244 and name CA)	12.37	0.92	0.93
	assign (segid 3A4 and resid 77 and name CB) (segid 3A4 and resid 244 and name CB)	13.04	0.94	0.94
40	assign (segid 3A4 and resid 77 and name CB) (segid 3A4 and resid 245 and name CA)	15.54	0.87	0.86
	assign (segid 3A4 and resid 77 and name CB) (segid 3A4 and resid 245 and name CB)	16.46	0.92	0.92
	assign (segid 3A4 and resid 77 and name CB) (segid 3A4 and resid 246 and name CA)	14.26	0.71	0.71
	assign (segid 3A4 and resid 77 and name CB) (segid 3A4 and resid 246 and name CB)	13.53	0.70	0.70
	assign (segid 3A4 and resid 77 and name CB) (segid 3A4 and resid 247 and name CA)	12.52	0.56	0.56
	assign (segid 3A4 and resid 77 and name CB) (segid 3A4 and resid 247 and name CB)	11.44	0.54	0.55
45	assign (segid 3A4 and resid 77 and name CB) (segid 3A4 and resid 248 and name CA)	15.81	0.57	0.57
	assign (segid 3A4 and resid 77 and name CB) (segid 3A4 and resid 248 and name CB)	16.49	0.65	0.64
	assign (segid 3A4 and resid 77 and name CB) (segid 3A4 and resid 249 and name CA)	17.80	0.61	0.61
	assign (segid 3A4 and resid 77 and name CB) (segid 3A4 and resid 250 and name CA)	16.24	0.54	0.54
	assign (segid 3A4 and resid 77 and name CB) (segid 3A4 and resid 250 and name CB)	14.88	0.58	0.58
50	assign (segid 3A4 and resid 77 and name CB) (segid 3A4 and resid 251 and name CA)	16.83	0.45	0.45
	assign (segid 3A4 and resid 77 and name CB) (segid 3A4 and resid 251 and name CB)	16.34	0.45	0.44
	assign (segid 3A4 and resid 77 and name CB) (segid 3A4 and resid 387 and name CA)	17.16	0.41	0.42
	assign (segid 3A4 and resid 77 and name CB) (segid 3A4 and resid 388 and name CA)	13.43	0.43	0.44
	assign (segid 3A4 and resid 77 and name CB) (segid 3A4 and resid 388 and name CB)	12.65	0.51	0.51
55	assign (segid 3A4 and resid 77 and name CB) (segid 3A4 and resid 389 and name CA)	13.85	0.28	0.27
	assign (segid 3A4 and resid 77 and name CB) (segid 3A4 and resid 389 and name CB)	14.31	0.26	0.27
	assign (segid 3A4 and resid 77 and name CB) (segid 3A4 and resid 390 and name CA)	16.43	0.32	0.31
	assign (segid 3A4 and resid 77 and name CB) (segid 3A4 and resid 390 and name CB)	16.86	0.42	0.42
60	assign (segid 3A4 and resid 77 and name CB) (segid 3A4 and resid 391 and name CA)	17.03	0.24	0.23
	assign (segid 3A4 and resid 77 and name CB) (segid 3A4 and resid 391 and name CB)	18.47	0.24	0.25
	assign (segid 3A4 and resid 77 and name CB) (segid 3A4 and resid 392 and name CA)	14.93	0.27	0.28
	assign (segid 3A4 and resid 77 and name CB) (segid 3A4 and resid 392 and name CB)	13.71	0.30	0.31
	assign (segid 3A4 and resid 77 and name CB) (segid 3A4 and resid 393 and name CA)	18.05	0.37	0.37
65	assign (segid 3A4 and resid 77 and name CB) (segid 3A4 and resid 78 and name C)	5.46	0.08	0.07
	assign (segid 3A4 and resid 77 and name CB) (segid 3A4 and resid 78 and name CA)	4.48	0.08	0.08
	assign (segid 3A4 and resid 77 and name CB) (segid 3A4 and resid 78 and name CB)	5.29	0.10	0.11
	assign (segid 3A4 and resid 77 and name CB) (segid 3A4 and resid 78 and name N)	3.14	0.08	0.08
	assign (segid 3A4 and resid 77 and name CB) (segid 3A4 and resid 78 and name O)	6.33	0.12	0.13
70	assign (segid 3A4 and resid 77 and name CB) (segid 3A4 and resid 79 and name C)	6.96	0.14	0.15
	assign (segid 3A4 and resid 77 and name CB) (segid 3A4 and resid 79 and name CA)	6.83	0.10	0.10
	assign (segid 3A4 and resid 77 and name CB) (segid 3A4 and resid 79 and name CB)	7.28	0.13	0.12
	assign (segid 3A4 and resid 77 and name CB) (segid 3A4 and resid 79 and name N)	5.62	0.11	0.11
	assign (segid 3A4 and resid 77 and name CB) (segid 3A4 and resid 90 and name C)	7.09	0.29	0.29
75	assign (segid 3A4 and resid 77 and name CB) (segid 3A4 and resid 80 and name CA)	6.57	0.28	0.28
	assign (segid 3A4 and resid 77 and name CB) (segid 3A4 and resid 80 and name N)	6.09	0.19	0.18
	assign (segid 3A4 and resid 77 and name CB) (segid 3A4 and resid 81 and name CA)	7.39	0.41	0.41
	assign (segid 3A4 and resid 77 and name CB) (segid 3A4 and resid 81 and name CB)	6.89	0.50	0.51
	assign (segid 3A4 and resid 77 and name CB) (segid 3A4 and resid 81 and name N)	6.53	0.38	0.38
80	assign (segid 3A4 and resid 77 and name CB) (segid 3A4 and resid 82 and name CA)	10.12	0.57	0.58
	assign (segid 3A4 and resid 77 and name CB) (segid 3A4 and resid 92 and name CB)	10.28	0.73	0.74
	assign (segid 3A4 and resid 77 and name CB) (segid 3A4 and resid 83 and name CA)	11.40	0.23	0.23
	assign (segid 3A4 and resid 77 and name CB) (segid 3A4 and resid 83 and name CB)	10.84	0.22	0.22

	assign (segid 3A4 and resid 77 and name CB) (segid 3A4 and resid 84 and name CA)	13.01	0.87	0.88
	assign (segid 3A4 and resid 77 and name CB) (segid 3A4 and resid 84 and name CB)	12.60	1.10	1.09
	assign (segid 3A4 and resid 77 and name CB) (segid 3A4 and resid 85 and name CA)	14.88	1.00	0.99
	assign (segid 3A4 and resid 77 and name CB) (segid 3A4 and resid 85 and name CB)	14.51	1.13	1.14
5	assign (segid 3A4 and resid 77 and name CB) (segid 3A4 and resid 86 and name CA)	15.96	0.62	0.62
	assign (segid 3A4 and resid 77 and name CB) (segid 3A4 and resid 86 and name CB)	15.41	0.60	0.59
	assign (segid 3A4 and resid 77 and name N) (segid 3A4 and resid 77 and name C)	2.45	0.02	0.03
	assign (segid 3A4 and resid 77 and name N) (segid 3A4 and resid 77 and name CA)	1.45	0.00	0.01
	assign (segid 3A4 and resid 77 and name N) (segid 3A4 and resid 77 and name CB)	2.44	0.05	0.04
10	assign (segid 3A4 and resid 77 and name N) (segid 3A4 and resid 77 and name O)	3.48	0.04	0.03
	assign (segid 3A4 and resid 77 and name N) (segid 3A4 and resid 78 and name C)	4.70	0.03	0.03
	assign (segid 3A4 and resid 77 and name N) (segid 3A4 and resid 78 and name CA)	4.24	0.06	0.05
	assign (segid 3A4 and resid 77 and name N) (segid 3A4 and resid 78 and name CB)	5.06	0.09	0.08
	assign (segid 3A4 and resid 77 and name N) (segid 3A4 and resid 78 and name N)	2.83	0.06	0.07
15	assign (segid 3A4 and resid 77 and name N) (segid 3A4 and resid 78 and name O)	5.75	0.07	0.07
	assign (segid 3A4 and resid 77 and name N) (segid 3A4 and resid 79 and name C)	5.57	0.05	0.06
	assign (segid 3A4 and resid 77 and name N) (segid 3A4 and resid 79 and name CA)	5.27	0.07	0.07
	assign (segid 3A4 and resid 77 and name N) (segid 3A4 and resid 79 and name CB)	5.32	0.13	0.13
	assign (segid 3A4 and resid 77 and name N) (segid 3A4 and resid 79 and name CG)	6.62	0.14	0.15
20	assign (segid 3A4 and resid 77 and name N) (segid 3A4 and resid 79 and name N)	4.29	0.08	0.07
	assign (segid 3A4 and resid 77 and name N) (segid 3A4 and resid 79 and name O)	6.78	0.07	0.06
	assign (segid 3A4 and resid 77 and name N) (segid 3A4 and resid 80 and name C)	6.46	0.12	0.12
	assign (segid 3A4 and resid 77 and name N) (segid 3A4 and resid 80 and name CA)	5.52	0.16	0.15
	assign (segid 3A4 and resid 77 and name N) (segid 3A4 and resid 80 and name N)	4.76	0.09	0.08
25	assign (segid 3A4 and resid 77 and name N) (segid 3A4 and resid 80 and name O)	7.62	0.12	0.11
	assign (segid 3A4 and resid 77 and name N) (segid 3A4 and resid 81 and name CA)	7.41	0.19	0.20
	assign (segid 3A4 and resid 77 and name N) (segid 3A4 and resid 81 and name CB)	7.30	0.27	0.27
	assign (segid 3A4 and resid 77 and name N) (segid 3A4 and resid 81 and name N)	6.22	0.18	0.18
	assign (segid 3A4 and resid 77 and name O) (segid 3A4 and resid 77 and name CB)	3.34	0.07	0.06
30	assign (segid 3A4 and resid 77 and name O) (segid 3A4 and resid 78 and name C)	3.05	0.09	0.10
	assign (segid 3A4 and resid 77 and name O) (segid 3A4 and resid 78 and name CA)	2.76	0.02	0.03
	assign (segid 3A4 and resid 77 and name O) (segid 3A4 and resid 78 and name CB)	4.23	0.04	0.04
	assign (segid 3A4 and resid 77 and name O) (segid 3A4 and resid 78 and name N)	2.26	0.01	0.01
	assign (segid 3A4 and resid 77 and name O) (segid 3A4 and resid 78 and name O)	3.51	0.18	0.17
35	assign (segid 3A4 and resid 77 and name O) (segid 3A4 and resid 79 and name C)	4.25	0.26	0.25
	assign (segid 3A4 and resid 77 and name O) (segid 3A4 and resid 79 and name CA)	4.51	0.21	0.21
	assign (segid 3A4 and resid 77 and name O) (segid 3A4 and resid 79 and name CB)	5.49	0.22	0.22
	assign (segid 3A4 and resid 77 and name O) (segid 3A4 and resid 79 and name CG)	6.70	0.22	0.22
	assign (segid 3A4 and resid 77 and name O) (segid 3A4 and resid 79 and name N)	3.54	0.18	0.19
40	assign (segid 3A4 and resid 77 and name O) (segid 3A4 and resid 79 and name O)	5.12	0.29	0.30
	assign (segid 3A4 and resid 77 and name O) (segid 3A4 and resid 80 and name C)	4.04	0.27	0.27
	assign (segid 3A4 and resid 77 and name O) (segid 3A4 and resid 80 and name CA)	3.90	0.26	0.26
	assign (segid 3A4 and resid 77 and name O) (segid 3A4 and resid 80 and name N)	3.48	0.23	0.23
	assign (segid 3A4 and resid 77 and name O) (segid 3A4 and resid 80 and name O)	5.19	0.22	0.23
45	assign (segid 3A4 and resid 77 and name O) (segid 3A4 and resid 81 and name C)	5.40	0.42	0.42
	assign (segid 3A4 and resid 77 and name O) (segid 3A4 and resid 81 and name CA)	4.19	0.33	0.32
	assign (segid 3A4 and resid 77 and name O) (segid 3A4 and resid 81 and name CB)	3.90	0.34	0.35
	assign (segid 3A4 and resid 77 and name O) (segid 3A4 and resid 81 and name N)	3.30	0.35	0.34
	assign (segid 3A4 and resid 77 and name O) (segid 3A4 and resid 81 and name O)	6.50	0.37	0.37
50	assign (segid 3A4 and resid 77 and name O) (segid 3A4 and resid 82 and name N)	5.49	0.55	0.54
	assign (segid 3A4 and resid 78 and name C) (segid 3A4 and resid 247 and name CB)	7.36	0.39	0.39
	assign (segid 3A4 and resid 78 and name C) (segid 3A4 and resid 78 and name CB)	2.51	0.02	0.03
	assign (segid 3A4 and resid 78 and name C) (segid 3A4 and resid 78 and name O)	1.23	0.00	0.00
	assign (segid 3A4 and resid 78 and name C) (segid 3A4 and resid 79 and name C)	3.02	0.04	0.05
55	assign (segid 3A4 and resid 78 and name C) (segid 3A4 and resid 79 and name CA)	2.43	0.01	0.01
	assign (segid 3A4 and resid 78 and name C) (segid 3A4 and resid 79 and name CB)	3.70	0.01	0.02
	assign (segid 3A4 and resid 78 and name C) (segid 3A4 and resid 79 and name CG)	4.97	0.03	0.03
	assign (segid 3A4 and resid 78 and name C) (segid 3A4 and resid 79 and name N)	1.33	0.01	0.01
	assign (segid 3A4 and resid 78 and name C) (segid 3A4 and resid 79 and name O)	3.84	0.09	0.09
60	assign (segid 3A4 and resid 78 and name C) (segid 3A4 and resid 80 and name C)	4.63	0.06	0.07
	assign (segid 3A4 and resid 78 and name C) (segid 3A4 and resid 80 and name CA)	4.49	0.11	0.11
	assign (segid 3A4 and resid 78 and name C) (segid 3A4 and resid 80 and name N)	3.32	0.12	0.12
	assign (segid 3A4 and resid 78 and name C) (segid 3A4 and resid 80 and name O)	5.73	0.10	0.10
	assign (segid 3A4 and resid 78 and name C) (segid 3A4 and resid 81 and name C)	5.16	0.24	0.24
65	assign (segid 3A4 and resid 78 and name C) (segid 3A4 and resid 81 and name CA)	4.70	0.05	0.05
	assign (segid 3A4 and resid 78 and name C) (segid 3A4 and resid 81 and name CB)	4.46	0.07	0.07
	assign (segid 3A4 and resid 78 and name C) (segid 3A4 and resid 81 and name N)	3.92	0.10	0.09
	assign (segid 3A4 and resid 78 and name C) (segid 3A4 and resid 81 and name O)	6.36	0.23	0.23
	assign (segid 3A4 and resid 78 and name C) (segid 3A4 and resid 82 and name C)	6.42	0.47	0.47
70	assign (segid 3A4 and resid 78 and name C) (segid 3A4 and resid 82 and name CA)	5.50	0.57	0.58
	assign (segid 3A4 and resid 78 and name C) (segid 3A4 and resid 82 and name CB)	5.20	0.77	0.77
	assign (segid 3A4 and resid 78 and name C) (segid 3A4 and resid 82 and name N)	4.53	0.44	0.44
	assign (segid 3A4 and resid 78 and name C) (segid 3A4 and resid 83 and name CA)	7.29	0.26	0.25
	assign (segid 3A4 and resid 78 and name C) (segid 3A4 and resid 83 and name CB)	7.16	0.16	0.16
75	assign (segid 3A4 and resid 78 and name C) (segid 3A4 and resid 83 and name N)	6.14	0.34	0.35
	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 134 and name CA)	19.22	0.39	0.40
	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 137 and name CA)	17.19	1.46	1.46
	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 138 and name CA)	16.99	0.49	0.49
	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 138 and name CB)	17.05	0.70	0.69
80	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 195 and name CA)	18.72	0.61	0.61
	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 195 and name CB)	18.67	0.65	0.64
	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 198 and name CA)	17.93	0.49	0.48
	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 198 and name CB)	16.73	0.51	0.52

	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 199 and name CA)	18.33	0.49	0.50
	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 199 and name CB)	18.95	0.57	0.57
	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 201 and name CB)	19.03	0.44	0.43
	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 202 and name CA)	16.82	0.34	0.33
5	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 202 and name CB)	15.84	0.31	0.32
	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 205 and name CA)	19.14	0.35	0.35
	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 205 and name CB)	17.93	0.31	0.32
	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 206 and name CA)	18.80	0.53	0.52
	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 206 and name CB)	18.52	0.57	0.57
10	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 219 and name CA)	16.84	0.91	0.91
	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 219 and name CB)	17.50	0.85	0.84
	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 220 and name CA)	13.22	0.93	0.93
	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 220 and name CB)	12.80	0.95	0.96
	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 221 and name CA)	13.51	0.67	0.67
	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 221 and name CB)	14.64	0.64	0.64
15	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 222 and name CA)	15.11	0.65	0.64
	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 222 and name CB)	16.37	0.66	0.66
	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 223 and name CA)	12.58	0.79	0.80
	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 223 and name CB)	12.25	0.92	0.93
20	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 224 and name CA)	9.84	0.61	0.62
	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 224 and name CB)	9.48	0.56	0.55
	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 225 and name CA)	12.60	0.57	0.58
	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 225 and name CB)	13.95	0.56	0.56
	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 226 and name CA)	13.63	0.70	0.69
25	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 240 and name CA)	11.02	0.64	0.64
	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 240 and name CB)	11.34	0.70	0.69
	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 241 and name CA)	12.97	0.50	0.50
	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 241 and name CB)	14.46	0.51	0.51
	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 242 and name CA)	12.50	0.55	0.55
30	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 242 and name CB)	13.01	0.60	0.60
	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 243 and name CA)	8.76	0.51	0.52
	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 243 and name CB)	7.79	0.56	0.56
	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 244 and name CA)	9.42	0.55	0.55
	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 244 and name CB)	10.34	0.54	0.54
35	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 245 and name CA)	12.27	0.51	0.52
	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 245 and name CB)	13.41	0.51	0.52
	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 246 and name CA)	10.79	0.41	0.41
	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 246 and name CB)	10.32	0.32	0.33
	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 247 and name CA)	8.45	0.43	0.42
40	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 247 and name CB)	7.38	0.44	0.43
	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 248 and name CA)	11.72	0.48	0.48
	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 248 and name CB)	12.55	0.51	0.51
	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 249 and name CA)	13.72	0.49	0.49
	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 250 and name CA)	12.03	0.41	0.41
45	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 250 and name CB)	10.71	0.42	0.43
	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 251 and name CA)	12.44	0.42	0.43
	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 251 and name CB)	11.96	0.45	0.44
	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 252 and name CA)	15.99	0.46	0.46
	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 252 and name CB)	16.46	0.47	0.47
50	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 253 and name CA)	17.02	0.49	0.48
	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 254 and name CA)	15.71	0.30	0.30
	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 255 and name CA)	17.16	0.66	0.66
	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 384 and name CA)	18.75	0.32	0.31
	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 384 and name CB)	18.47	0.33	0.32
55	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 385 and name CA)	18.16	0.43	0.42
	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 386 and name CA)	17.92	0.30	0.29
	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 387 and name CA)	15.91	0.23	0.22
	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 388 and name CA)	12.31	0.32	0.33
	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 388 and name CB)	11.91	0.44	0.45
60	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 389 and name CA)	11.69	0.31	0.32
	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 389 and name CB)	12.17	0.39	0.39
	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 390 and name CA)	13.94	0.31	0.31
	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 390 and name CB)	14.58	0.35	0.36
	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 391 and name CA)	13.75	0.32	0.32
65	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 391 and name CB)	15.09	0.32	0.32
	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 392 and name CA)	11.48	0.38	0.39
	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 392 and name CB)	10.10	0.43	0.44
	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 393 and name CA)	14.26	0.53	0.54
	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 394 and name CA)	17.08	0.47	0.47
	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 394 and name CB)	17.09	0.46	0.47
70	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 395 and name CA)	18.32	0.64	0.64
	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 396 and name CA)	18.51	0.69	0.69
	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 396 and name CB)	17.46	0.71	0.71
	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 78 and name C)	1.52	0.01	0.01
75	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 78 and name CB)	1.52	0.01	0.02
	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 79 and name C)	2.40	0.02	0.01
	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 79 and name CA)	4.41	0.04	0.04
	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 79 and name CB)	3.81	0.02	0.01
	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 79 and name CG)	4.96	0.04	0.03
80	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 79 and name N)	6.25	0.03	0.03
	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 79 and name O)	2.44	0.02	0.01
	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 80 and name C)	5.29	0.10	0.10
	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 80 and name C)	5.58	0.07	0.07

	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 80 and name CA)	5.46	0.11	0.11
	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 80 and name N)	4.41	0.11	0.10
	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 80 and name O)	6.73	0.09	0.08
	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 81 and name C)	6.05	0.31	0.30
5	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 81 and name CA)	5.34	0.10	0.10
	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 81 and name CB)	4.74	0.08	0.07
	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 81 and name N)	4.70	0.08	0.08
	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 81 and name O)	7.21	0.27	0.28
	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 82 and name CA)	6.67	0.64	0.65
	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 82 and name CB)	6.40	0.83	0.82
10	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 82 and name N)	5.62	0.52	0.51
	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 83 and name CA)	8.71	0.26	0.26
	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 83 and name CB)	8.58	0.14	0.14
	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 84 and name CA)	10.95	0.71	0.70
	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 84 and name CB)	10.88	0.87	0.87
15	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 85 and name CA)	12.01	0.95	0.95
	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 85 and name CB)	11.48	1.05	1.06
	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 86 and name CA)	12.65	0.76	0.76
	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 86 and name CB)	11.89	0.73	0.74
	assign (segid 3A4 and resid 78 and name CA) (segid 3A4 and resid 134 and name CA)	19.00	0.54	0.54
20	assign (segid 3A4 and resid 78 and name CB) (segid 3A4 and resid 137 and name CA)	17.25	1.68	1.68
	assign (segid 3A4 and resid 78 and name CB) (segid 3A4 and resid 138 and name CA)	16.92	0.55	0.55
	assign (segid 3A4 and resid 78 and name CB) (segid 3A4 and resid 138 and name CB)	16.85	0.74	0.75
	assign (segid 3A4 and resid 78 and name CB) (segid 3A4 and resid 195 and name CA)	17.66	0.68	0.68
	assign (segid 3A4 and resid 78 and name CB) (segid 3A4 and resid 195 and name CB)	17.54	0.68	0.69
25	assign (segid 3A4 and resid 78 and name CB) (segid 3A4 and resid 198 and name CA)	17.20	0.59	0.59
	assign (segid 3A4 and resid 78 and name CB) (segid 3A4 and resid 198 and name CB)	15.95	0.62	0.61
	assign (segid 3A4 and resid 78 and name CB) (segid 3A4 and resid 199 and name CA)	17.62	0.58	0.58
	assign (segid 3A4 and resid 78 and name CB) (segid 3A4 and resid 199 and name CB)	18.16	0.65	0.65
30	assign (segid 3A4 and resid 78 and name CB) (segid 3A4 and resid 201 and name CA)	19.21	0.43	0.44
	assign (segid 3A4 and resid 78 and name CB) (segid 3A4 and resid 201 and name CB)	18.61	0.49	0.50
	assign (segid 3A4 and resid 78 and name CB) (segid 3A4 and resid 202 and name CA)	16.50	0.38	0.38
	assign (segid 3A4 and resid 78 and name CB) (segid 3A4 and resid 202 and name CB)	15.44	0.38	0.38
	assign (segid 3A4 and resid 78 and name CB) (segid 3A4 and resid 205 and name CA)	19.18	0.37	0.37
35	assign (segid 3A4 and resid 78 and name CB) (segid 3A4 and resid 205 and name CB)	17.96	0.34	0.34
	assign (segid 3A4 and resid 78 and name CB) (segid 3A4 and resid 206 and name CA)	18.90	0.53	0.54
	assign (segid 3A4 and resid 78 and name CB) (segid 3A4 and resid 206 and name CB)	18.55	0.58	0.58
	assign (segid 3A4 and resid 78 and name CB) (segid 3A4 and resid 219 and name CA)	17.21	0.99	1.00
	assign (segid 3A4 and resid 78 and name CB) (segid 3A4 and resid 219 and name CB)	17.76	0.95	0.95
40	assign (segid 3A4 and resid 78 and name CB) (segid 3A4 and resid 220 and name CA)	13.53	1.04	1.04
	assign (segid 3A4 and resid 78 and name CB) (segid 3A4 and resid 220 and name CB)	13.02	1.10	1.09
	assign (segid 3A4 and resid 78 and name CB) (segid 3A4 and resid 221 and name CA)	13.59	0.77	0.77
	assign (segid 3A4 and resid 78 and name CB) (segid 3A4 and resid 221 and name CB)	14.61	0.75	0.75
	assign (segid 3A4 and resid 78 and name CB) (segid 3A4 and resid 222 and name CA)	15.48	0.71	0.70
45	assign (segid 3A4 and resid 78 and name CB) (segid 3A4 and resid 222 and name CB)	16.79	0.72	0.72
	assign (segid 3A4 and resid 78 and name CB) (segid 3A4 and resid 223 and name CA)	13.73	0.85	0.85
	assign (segid 3A4 and resid 78 and name CB) (segid 3A4 and resid 223 and name CB)	12.96	0.98	0.98
	assign (segid 3A4 and resid 78 and name CB) (segid 3A4 and resid 224 and name CA)	10.26	0.68	0.68
	assign (segid 3A4 and resid 78 and name CB) (segid 3A4 and resid 224 and name CB)	9.70	0.63	0.64
50	assign (segid 3A4 and resid 78 and name CB) (segid 3A4 and resid 225 and name CA)	12.88	0.60	0.60
	assign (segid 3A4 and resid 78 and name CB) (segid 3A4 and resid 225 and name CB)	14.17	0.60	0.60
	assign (segid 3A4 and resid 78 and name CB) (segid 3A4 and resid 226 and name CA)	14.26	0.72	0.72
	assign (segid 3A4 and resid 78 and name CB) (segid 3A4 and resid 240 and name CA)	10.62	0.51	0.51
	assign (segid 3A4 and resid 78 and name CB) (segid 3A4 and resid 240 and name CB)	10.81	0.58	0.57
55	assign (segid 3A4 and resid 78 and name CB) (segid 3A4 and resid 241 and name CA)	12.40	0.47	0.48
	assign (segid 3A4 and resid 78 and name CB) (segid 3A4 and resid 241 and name CB)	13.89	0.48	0.48
	assign (segid 3A4 and resid 78 and name CB) (segid 3A4 and resid 242 and name CA)	11.55	0.55	0.54
	assign (segid 3A4 and resid 78 and name CB) (segid 3A4 and resid 242 and name CB)	12.01	0.57	0.56
	assign (segid 3A4 and resid 78 and name CB) (segid 3A4 and resid 243 and name CA)	7.80	0.52	0.52
60	assign (segid 3A4 and resid 78 and name CB) (segid 3A4 and resid 243 and name CB)	6.93	0.53	0.53
	assign (segid 3A4 and resid 78 and name CB) (segid 3A4 and resid 244 and name CA)	8.83	0.66	0.66
	assign (segid 3A4 and resid 78 and name CB) (segid 3A4 and resid 244 and name CB)	9.90	0.63	0.64
	assign (segid 3A4 and resid 78 and name CB) (segid 3A4 and resid 245 and name CA)	11.40	0.62	0.61
	assign (segid 3A4 and resid 78 and name CB) (segid 3A4 and resid 245 and name CB)	12.48	0.61	0.61
65	assign (segid 3A4 and resid 78 and name CB) (segid 3A4 and resid 246 and name CA)	9.61	0.49	0.50
	assign (segid 3A4 and resid 78 and name CB) (segid 3A4 and resid 246 and name CB)	9.05	0.41	0.40
	assign (segid 3A4 and resid 78 and name CB) (segid 3A4 and resid 247 and name CA)	7.55	0.54	0.53
	assign (segid 3A4 and resid 78 and name CB) (segid 3A4 and resid 247 and name CB)	6.65	0.55	0.55
	assign (segid 3A4 and resid 78 and name CB) (segid 3A4 and resid 248 and name CA)	11.05	0.58	0.58
70	assign (segid 3A4 and resid 78 and name CB) (segid 3A4 and resid 248 and name CB)	11.93	0.62	0.61
	assign (segid 3A4 and resid 78 and name CB) (segid 3A4 and resid 249 and name CA)	12.75	0.57	0.57
	assign (segid 3A4 and resid 78 and name CB) (segid 3A4 and resid 250 and name CA)	11.05	0.46	0.47
	assign (segid 3A4 and resid 78 and name CB) (segid 3A4 and resid 250 and name CB)	9.70	0.47	0.46
	assign (segid 3A4 and resid 78 and name CB) (segid 3A4 and resid 251 and name CA)	11.86	0.49	0.49
75	assign (segid 3A4 and resid 78 and name CB) (segid 3A4 and resid 251 and name CB)	11.51	0.50	0.49
	assign (segid 3A4 and resid 78 and name CB) (segid 3A4 and resid 252 and name CA)	15.31	0.53	0.53
	assign (segid 3A4 and resid 78 and name CB) (segid 3A4 and resid 252 and name CB)	15.73	0.54	0.55
	assign (segid 3A4 and resid 78 and name CB) (segid 3A4 and resid 253 and name CA)	16.14	0.55	0.54
	assign (segid 3A4 and resid 78 and name CB) (segid 3A4 and resid 254 and name CA)	14.97	0.39	0.39
80	assign (segid 3A4 and resid 78 and name CB) (segid 3A4 and resid 255 and name CA)	16.66	0.75	0.74
	assign (segid 3A4 and resid 78 and name CB) (segid 3A4 and resid 384 and name CA)	18.56	0.39	0.39
	assign (segid 3A4 and resid 78 and name CB) (segid 3A4 and resid 384 and name CB)	18.39	0.37	0.37
	assign (segid 3A4 and resid 78 and name CB) (segid 3A4 and resid 385 and name CA)	17.89	0.57	0.57

	assign (segid 3A4 and resid 78 and name CB)	(segid 3A4 and resid 386 and name CA)	17.85	0.46	0.45
	assign (segid 3A4 and resid 78 and name CB)	(segid 3A4 and resid 387 and name CA)	15.96	0.39	0.39
	assign (segid 3A4 and resid 78 and name CB)	(segid 3A4 and resid 388 and name CA)	12.43	0.51	0.51
	assign (segid 3A4 and resid 78 and name CB)	(segid 3A4 and resid 388 and name CB)	12.02	0.65	0.65
	assign (segid 3A4 and resid 78 and name CB)	(segid 3A4 and resid 389 and name CA)	11.48	0.44	0.43
5	assign (segid 3A4 and resid 78 and name CB)	(segid 3A4 and resid 389 and name CB)	11.78	0.51	0.51
	assign (segid 3A4 and resid 78 and name CB)	(segid 3A4 and resid 390 and name CA)	13.91	0.38	0.37
	assign (segid 3A4 and resid 78 and name CB)	(segid 3A4 and resid 390 and name CB)	14.68	0.41	0.41
	assign (segid 3A4 and resid 78 and name CB)	(segid 3A4 and resid 391 and name CA)	13.64	0.36	0.36
	assign (segid 3A4 and resid 78 and name CB)	(segid 3A4 and resid 391 and name CB)	14.95	0.36	0.36
10	assign (segid 3A4 and resid 78 and name CB)	(segid 3A4 and resid 392 and name CA)	11.65	0.47	0.47
	assign (segid 3A4 and resid 78 and name CB)	(segid 3A4 and resid 392 and name CB)	10.23	0.53	0.54
	assign (segid 3A4 and resid 78 and name CB)	(segid 3A4 and resid 393 and name CA)	14.34	0.65	0.65
	assign (segid 3A4 and resid 78 and name CB)	(segid 3A4 and resid 394 and name CA)	17.23	0.54	0.54
	assign (segid 3A4 and resid 78 and name CB)	(segid 3A4 and resid 394 and name CB)	17.29	0.51	0.51
15	assign (segid 3A4 and resid 78 and name CB)	(segid 3A4 and resid 395 and name CA)	18.71	0.69	0.70
	assign (segid 3A4 and resid 78 and name CB)	(segid 3A4 and resid 396 and name CA)	18.76	0.80	0.80
	assign (segid 3A4 and resid 78 and name CB)	(segid 3A4 and resid 396 and name CB)	17.68	0.84	0.84
	assign (segid 3A4 and resid 78 and name CB)	(segid 3A4 and resid 79 and name C)	5.46	0.08	0.09
	assign (segid 3A4 and resid 78 and name CB)	(segid 3A4 and resid 79 and name CA)	4.53	0.10	0.10
20	assign (segid 3A4 and resid 78 and name CB)	(segid 3A4 and resid 79 and name CB)	5.39	0.12	0.13
	assign (segid 3A4 and resid 78 and name CB)	(segid 3A4 and resid 79 and name CG)	6.81	0.14	0.13
	assign (segid 3A4 and resid 78 and name CB)	(segid 3A4 and resid 79 and name N)	3.20	0.09	0.10
	assign (segid 3A4 and resid 78 and name CB)	(segid 3A4 and resid 79 and name O)	6.30	0.10	0.10
	assign (segid 3A4 and resid 78 and name CB)	(segid 3A4 and resid 80 and name C)	6.99	0.06	0.06
25	assign (segid 3A4 and resid 78 and name CB)	(segid 3A4 and resid 80 and name CA)	6.84	0.11	0.12
	assign (segid 3A4 and resid 78 and name CB)	(segid 3A4 and resid 80 and name N)	5.67	0.13	0.14
	assign (segid 3A4 and resid 78 and name CB)	(segid 3A4 and resid 80 and name C)	7.17	0.28	0.29
	assign (segid 3A4 and resid 78 and name CB)	(segid 3A4 and resid 81 and name CA)	6.64	0.08	0.08
	assign (segid 3A4 and resid 78 and name CB)	(segid 3A4 and resid 81 and name CB)	5.91	0.07	0.07
30	assign (segid 3A4 and resid 78 and name CB)	(segid 3A4 and resid 81 and name N)	6.10	0.07	0.07
	assign (segid 3A4 and resid 78 and name CB)	(segid 3A4 and resid 82 and name CA)	7.46	0.68	0.69
	assign (segid 3A4 and resid 78 and name CB)	(segid 3A4 and resid 82 and name CB)	6.92	0.88	0.88
	assign (segid 3A4 and resid 78 and name CB)	(segid 3A4 and resid 82 and name N)	6.61	0.51	0.51
	assign (segid 3A4 and resid 78 and name CB)	(segid 3A4 and resid 83 and name CA)	9.67	0.32	0.31
35	assign (segid 3A4 and resid 78 and name CB)	(segid 3A4 and resid 83 and name CB)	9.62	0.20	0.20
	assign (segid 3A4 and resid 78 and name CB)	(segid 3A4 and resid 84 and name CA)	12.09	0.69	0.70
	assign (segid 3A4 and resid 78 and name CB)	(segid 3A4 and resid 84 and name CB)	12.11	0.86	0.86
	assign (segid 3A4 and resid 78 and name CB)	(segid 3A4 and resid 85 and name CA)	12.87	0.98	0.98
	assign (segid 3A4 and resid 78 and name CB)	(segid 3A4 and resid 85 and name CB)	12.26	1.09	1.09
40	assign (segid 3A4 and resid 78 and name CB)	(segid 3A4 and resid 86 and name CA)	13.28	0.83	0.83
	assign (segid 3A4 and resid 78 and name CB)	(segid 3A4 and resid 86 and name CB)	12.41	0.82	0.82
	assign (segid 3A4 and resid 78 and name CB)	(segid 3A4 and resid 78 and name C)	2.46	0.02	0.02
	assign (segid 3A4 and resid 78 and name N)	(segid 3A4 and resid 78 and name CA)	1.47	0.01	0.01
	assign (segid 3A4 and resid 78 and name N)	(segid 3A4 and resid 78 and name CB)	2.47	0.02	0.01
45	assign (segid 3A4 and resid 78 and name N)	(segid 3A4 and resid 78 and name C)	3.50	0.06	0.06
	assign (segid 3A4 and resid 78 and name N)	(segid 3A4 and resid 79 and name C)	4.71	0.06	0.05
	assign (segid 3A4 and resid 78 and name N)	(segid 3A4 and resid 79 and name CA)	4.21	0.02	0.01
	assign (segid 3A4 and resid 78 and name N)	(segid 3A4 and resid 79 and name CB)	4.94	0.03	0.03
	assign (segid 3A4 and resid 78 and name N)	(segid 3A4 and resid 79 and name CG)	6.40	0.03	0.03
50	assign (segid 3A4 and resid 78 and name N)	(segid 3A4 and resid 79 and name N)	2.80	0.03	0.03
	assign (segid 3A4 and resid 78 and name N)	(segid 3A4 and resid 79 and name O)	5.77	0.09	0.09
	assign (segid 3A4 and resid 78 and name N)	(segid 3A4 and resid 80 and name C)	5.73	0.12	0.12
	assign (segid 3A4 and resid 78 and name N)	(segid 3A4 and resid 80 and name CA)	5.33	0.15	0.15
	assign (segid 3A4 and resid 78 and name N)	(segid 3A4 and resid 80 and name N)	4.34	0.13	0.12
55	assign (segid 3A4 and resid 78 and name N)	(segid 3A4 and resid 80 and name O)	6.93	0.11	0.11
	assign (segid 3A4 and resid 78 and name N)	(segid 3A4 and resid 81 and name C)	6.81	0.32	0.31
	assign (segid 3A4 and resid 78 and name N)	(segid 3A4 and resid 81 and name CA)	5.88	0.19	0.18
	assign (segid 3A4 and resid 78 and name N)	(segid 3A4 and resid 81 and name CB)	5.38	0.21	0.22
	assign (segid 3A4 and resid 78 and name N)	(segid 3A4 and resid 81 and name N)	5.01	0.15	0.15
60	assign (segid 3A4 and resid 78 and name N)	(segid 3A4 and resid 82 and name N)	6.52	0.48	0.48
	assign (segid 3A4 and resid 78 and name O)	(segid 3A4 and resid 247 and name CB)	6.84	0.54	0.55
	assign (segid 3A4 and resid 78 and name O)	(segid 3A4 and resid 78 and name CB)	3.30	0.09	0.08
	assign (segid 3A4 and resid 78 and name O)	(segid 3A4 and resid 79 and name C)	2.95	0.09	0.10
	assign (segid 3A4 and resid 78 and name O)	(segid 3A4 and resid 79 and name CA)	2.74	0.02	0.03
65	assign (segid 3A4 and resid 78 and name O)	(segid 3A4 and resid 79 and name CB)	4.23	0.02	0.02
	assign (segid 3A4 and resid 78 and name O)	(segid 3A4 and resid 79 and name CG)	5.24	0.04	0.05
	assign (segid 3A4 and resid 78 and name O)	(segid 3A4 and resid 79 and name N)	2.24	0.01	0.02
	assign (segid 3A4 and resid 78 and name O)	(segid 3A4 and resid 79 and name O)	3.40	0.11	0.10
	assign (segid 3A4 and resid 78 and name O)	(segid 3A4 and resid 80 and name C)	4.18	0.19	0.19
70	assign (segid 3A4 and resid 78 and name O)	(segid 3A4 and resid 80 and name CA)	4.40	0.23	0.22
	assign (segid 3A4 and resid 78 and name O)	(segid 3A4 and resid 80 and name N)	3.45	0.21	0.21
	assign (segid 3A4 and resid 78 and name O)	(segid 3A4 and resid 80 and name O)	5.14	0.14	0.14
	assign (segid 3A4 and resid 78 and name O)	(segid 3A4 and resid 81 and name C)	4.13	0.23	0.23
	assign (segid 3A4 and resid 78 and name O)	(segid 3A4 and resid 81 and name CA)	3.89	0.20	0.19
75	assign (segid 3A4 and resid 78 and name O)	(segid 3A4 and resid 81 and name CB)	3.70	0.28	0.27
	assign (segid 3A4 and resid 78 and name O)	(segid 3A4 and resid 81 and name N)	3.36	0.27	0.27
	assign (segid 3A4 and resid 78 and name O)	(segid 3A4 and resid 81 and name O)	5.30	0.22	0.21
	assign (segid 3A4 and resid 78 and name O)	(segid 3A4 and resid 82 and name C)	5.39	0.53	0.52
	assign (segid 3A4 and resid 78 and name O)	(segid 3A4 and resid 82 and name CA)	1.37	0.61	0.60
80	assign (segid 3A4 and resid 78 and name O)	(segid 3A4 and resid 82 and name CB)	1.12	0.78	0.77
	assign (segid 3A4 and resid 78 and name O)	(segid 3A4 and resid 82 and name N)	3.43	0.45	0.45
	assign (segid 3A4 and resid 78 and name O)	(segid 3A4 and resid 82 and name O)	6.53	0.54	0.55

	assign (segid 3A4 and resid 78 and name O) (segid 3A4 and resid 83 and name CA)	6.52	0.36	0.36
	assign (segid 3A4 and resid 78 and name O) (segid 3A4 and resid 83 and name CB)	6.60	0.27	0.26
	assign (segid 3A4 and resid 78 and name O) (segid 3A4 and resid 83 and name N)	5.26	0.42	0.42
	assign (segid 3A4 and resid 79 and name C) (segid 3A4 and resid 392 and name CB)	7.26	0.36	0.36
5	assign (segid 3A4 and resid 79 and name C) (segid 3A4 and resid 79 and name CB)	2.54	0.04	0.03
	assign (segid 3A4 and resid 79 and name C) (segid 3A4 and resid 79 and name CG)	3.02	0.06	0.06
	assign (segid 3A4 and resid 79 and name C) (segid 3A4 and resid 79 and name O)	1.24	0.01	0.01
	assign (segid 3A4 and resid 79 and name C) (segid 3A4 and resid 80 and name C)	3.02	0.07	0.06
	assign (segid 3A4 and resid 79 and name C) (segid 3A4 and resid 80 and name CA)	2.45	0.01	0.01
10	assign (segid 3A4 and resid 79 and name C) (segid 3A4 and resid 80 and name N)	1.33	0.00	0.01
	assign (segid 3A4 and resid 79 and name C) (segid 3A4 and resid 80 and name O)	3.88	0.17	0.16
	assign (segid 3A4 and resid 79 and name C) (segid 3A4 and resid 81 and name C)	4.58	0.10	0.10
	assign (segid 3A4 and resid 79 and name C) (segid 3A4 and resid 81 and name CA)	4.42	0.07	0.07
	assign (segid 3A4 and resid 79 and name C) (segid 3A4 and resid 81 and name CB)	5.14	0.13	0.13
15	assign (segid 3A4 and resid 79 and name C) (segid 3A4 and resid 81 and name N)	3.23	0.08	0.09
	assign (segid 3A4 and resid 79 and name C) (segid 3A4 and resid 81 and name O)	5.68	0.13	0.13
	assign (segid 3A4 and resid 79 and name C) (segid 3A4 and resid 82 and name C)	4.93	0.13	0.14
	assign (segid 3A4 and resid 79 and name C) (segid 3A4 and resid 82 and name CA)	4.73	0.23	0.23
	assign (segid 3A4 and resid 79 and name C) (segid 3A4 and resid 82 and name CB)	4.82	0.43	0.42
20	assign (segid 3A4 and resid 79 and name C) (segid 3A4 and resid 82 and name N)	3.90	0.16	0.17
	assign (segid 3A4 and resid 79 and name C) (segid 3A4 and resid 82 and name O)	6.12	0.12	0.12
	assign (segid 3A4 and resid 79 and name C) (segid 3A4 and resid 83 and name C)	6.16	0.09	0.10
	assign (segid 3A4 and resid 79 and name C) (segid 3A4 and resid 83 and name CA)	4.89	0.05	0.05
	assign (segid 3A4 and resid 79 and name C) (segid 3A4 and resid 83 and name CB)	4.39	0.12	0.12
25	assign (segid 3A4 and resid 79 and name C) (segid 3A4 and resid 83 and name N)	4.12	0.08	0.07
	assign (segid 3A4 and resid 79 and name C) (segid 3A4 and resid 83 and name O)	7.20	0.05	0.05
	assign (segid 3A4 and resid 79 and name C) (segid 3A4 and resid 84 and name N)	6.36	0.31	0.30
	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 137 and name CA)	16.55	0.74	0.74
30	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 138 and name CA)	17.01	1.02	1.02
	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 138 and name CB)	17.15	1.15	1.15
	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 198 and name CB)	18.24	0.44	0.44
	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 202 and name CB)	18.84	0.42	0.42
	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 202 and name CB)	18.02	0.33	0.33
35	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 219 and name CA)	16.75	0.68	0.68
	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 219 and name CB)	17.54	0.58	0.59
	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 220 and name CA)	13.18	0.57	0.58
	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 220 and name CB)	12.55	0.57	0.58
	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 221 and name CA)	14.43	0.20	0.21
40	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 221 and name CB)	15.63	0.20	0.19
	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 222 and name CA)	16.18	0.31	0.32
	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 222 and name CB)	17.25	0.36	0.37
	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 223 and name CA)	13.34	0.52	0.52
	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 223 and name CB)	12.61	0.66	0.65
45	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 224 and name CA)	11.35	0.32	0.32
	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 224 and name CB)	10.98	0.37	0.36
	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 225 and name CA)	14.70	0.43	0.42
	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 225 and name CB)	15.95	0.35	0.35
	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 226 and name CA)	15.52	0.52	0.53
50	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 240 and name CA)	14.52	0.50	0.50
	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 240 and name CB)	14.91	0.57	0.56
	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 241 and name CA)	16.10	0.26	0.25
	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 241 and name CB)	17.58	0.27	0.27
	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 242 and name CA)	15.52	0.36	0.36
	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 242 and name CB)	16.13	0.44	0.44
55	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 243 and name CA)	11.77	0.37	0.36
	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 243 and name CB)	11.04	0.43	0.42
	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 244 and name CA)	11.92	0.21	0.20
	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 244 and name CB)	12.88	0.14	0.14
60	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 245 and name CA)	14.37	0.30	0.30
	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 245 and name CB)	15.67	0.26	0.25
	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 246 and name CA)	12.58	0.31	0.31
	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 246 and name CB)	12.33	0.27	0.26
	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 247 and name CA)	9.59	0.41	0.42
65	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 247 and name CB)	8.70	0.41	0.40
	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 248 and name CA)	12.49	0.54	0.53
	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 248 and name CB)	13.58	0.51	0.51
	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 249 and name CA)	14.36	0.57	0.57
	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 250 and name CA)	11.93	0.58	0.58
70	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 250 and name CB)	10.64	0.59	0.59
	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 251 and name CA)	11.69	0.61	0.60
	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 251 and name CB)	11.31	0.65	0.65
	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 252 and name CA)	15.47	0.60	0.59
	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 252 and name CB)	16.26	0.61	0.61
75	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 253 and name CA)	16.35	0.56	0.56
	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 254 and name CA)	14.32	0.46	0.46
	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 255 and name CA)	15.52	0.51	0.51
	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 256 and name CA)	18.94	0.54	0.54
	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 258 and name CB)	18.15	0.58	0.58
80	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 319 and name CB)	18.61	0.23	0.24
	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 322 and name CA)	18.53	0.62	0.62
	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 323 and name CA)	18.01	0.90	0.91
	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 323 and name CB)	18.02	0.93	0.92
	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 383 and name CA)	19.27	0.32	0.31

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	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 384 and name CA)	15.55	0.29	0.30
	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 384 and name CB)	15.15	0.32	0.32
	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 385 and name CA)	15.11	0.33	0.32
	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 386 and name CA)	14.75	0.24	0.24
5	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 387 and name CA)	12.90	0.23	0.22
	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 388 and name CA)	9.46	0.26	0.25
	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 388 and name CB)	9.37	0.33	0.34
	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 388 and name O)	7.43	0.22	0.22
	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 389 and name CA)	8.93	0.24	0.24
10	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 389 and name CB)	9.73	0.27	0.26
	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 390 and name CA)	10.64	0.34	0.35
	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 390 and name CB)	11.14	0.39	0.40
	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 391 and name CA)	10.56	0.32	0.33
	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 391 and name CB)	11.96	0.33	0.32
15	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 392 and name CA)	8.22	0.24	0.23
	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 392 and name CB)	7.00	0.24	0.23
	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 393 and name CA)	11.39	0.25	0.25
	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 394 and name CA)	13.80	0.30	0.31
	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 394 and name CB)	13.68	0.31	0.33
20	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 395 and name CA)	15.10	0.41	0.40
	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 396 and name CA)	15.77	0.33	0.33
	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 396 and name CB)	14.90	0.35	0.36
	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 397 and name CA)	17.34	0.36	0.35
	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 397 and name CB)	16.81	0.38	0.37
25	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 398 and name CB)	19.31	0.37	0.36
	assign (segid 3A4 and resid 79 and name CA) (segid HEM and resid 1 and name CBD)	7.20	0.37	0.36
	assign (segid 3A4 and resid 79 and name CA) (segid HEM and resid 1 and name CGD)	6.70	0.39	0.39
	assign (segid 3A4 and resid 79 and name CA) (segid HEM and resid 1 and name OLD)	6.04	0.61	0.60
	assign (segid 3A4 and resid 79 and name CA) (segid HEM and resid 1 and name O2D)	7.24	0.58	0.58
30	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 79 and name C)	1.52	0.01	0.01
	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 79 and name CB)	1.54	0.02	0.01
	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 79 and name CG)	2.56	0.03	0.03
	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 79 and name O)	2.42	0.04	0.05
	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 80 and name C)	4.43	0.06	0.06
35	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 80 and name CA)	3.81	0.02	0.03
	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 80 and name N)	2.43	0.02	0.03
	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 80 and name O)	5.35	0.16	0.17
	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 81 and name C)	5.61	0.13	0.12
	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 81 and name CA)	5.46	0.07	0.07
40	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 81 and name CB)	5.85	0.15	0.15
	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 81 and name N)	4.37	0.08	0.08
	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 81 and name O)	6.75	0.15	0.16
	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 82 and name C)	5.81	0.23	0.24
	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 82 and name CA)	5.43	0.34	0.34
45	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 82 and name CB)	5.10	0.58	0.57
	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 82 and name N)	4.75	0.21	0.22
	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 82 and name O)	6.96	0.21	0.22
	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 83 and name C)	7.34	0.12	0.11
	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 83 and name CA)	5.96	0.11	0.11
50	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 83 and name CB)	5.55	0.11	0.12
	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 83 and name N)	5.16	0.16	0.15
	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 84 and name CA)	9.03	0.34	0.34
	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 84 and name CB)	9.37	0.47	0.46
	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 85 and name CA)	10.50	0.38	0.38
55	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 85 and name CB)	10.37	0.41	0.41
	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 86 and name CA)	10.32	0.27	0.27
	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 86 and name CB)	9.47	0.35	0.36
	assign (segid 3A4 and resid 79 and name CA) (segid 3A4 and resid 94 and name CB)	18.10	1.12	1.12
	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 137 and name CA)	17.59	0.66	0.67
60	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 202 and name CB)	19.38	0.31	0.30
	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 219 and name CA)	18.05	0.68	0.67
	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 219 and name CB)	18.84	0.58	0.58
	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 220 and name CA)	14.50	0.56	0.56
	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 220 and name CB)	13.80	0.57	0.56
65	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 221 and name CA)	15.84	0.22	0.22
	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 221 and name CB)	17.00	0.23	0.23
	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 222 and name CA)	17.66	0.30	0.29
	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 222 and name CB)	18.71	0.34	0.35
	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 223 and name CA)	14.80	0.49	0.49
70	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 223 and name CB)	14.03	0.62	0.62
	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 224 and name CA)	12.86	0.31	0.31
	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 224 and name CB)	12.45	0.37	0.37
	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 225 and name CA)	16.19	0.42	0.43
	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 225 and name CB)	17.45	0.36	0.35
75	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 226 and name CA)	17.01	0.51	0.51
	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 240 and name CA)	15.68	0.54	0.55
	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 240 and name CB)	15.97	0.62	0.61
	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 241 and name CA)	17.32	0.29	0.29
	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 241 and name CB)	18.81	0.30	0.30
80	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 242 and name CA)	16.53	0.39	0.39
	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 242 and name CB)	17.05	0.48	0.49
	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 243 and name CA)	12.77	0.38	0.39
	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 243 and name CB)	12.05	0.46	0.47

	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 244 and name CA)	13.18	0.22	0.21
	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 244 and name CB)	14.21	0.16	0.16
	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 245 and name CA)	15.47	0.28	0.28
	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 245 and name CB)	16.73	0.23	0.24
	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 246 and name CA)	13.41	0.29	0.29
5	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 246 and name CB)	13.07	0.24	0.24
	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 247 and name CA)	10.56	0.40	0.40
	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 247 and name CB)	9.81	0.39	0.38
	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 248 and name CA)	13.53	0.54	0.55
	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 248 and name CB)	14.70	0.50	0.51
10	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 249 and name CA)	15.13	0.57	0.56
	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 250 and name CA)	12.43	0.59	0.60
	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 250 and name CB)	11.10	0.59	0.59
	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 251 and name CA)	12.34	0.66	0.66
	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 251 and name CB)	12.11	0.71	0.71
15	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 252 and name CA)	16.11	0.64	0.65
	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 252 and name CB)	16.98	0.64	0.63
	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 253 and name CA)	16.70	0.58	0.58
	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 254 and name CA)	14.44	0.53	0.53
	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 255 and name CA)	15.78	0.57	0.57
20	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 258 and name CB)	17.97	0.50	0.51
	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 319 and name CB)	17.97	0.33	0.32
	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 322 and name CA)	17.52	0.62	0.63
	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 323 and name CA)	16.89	0.93	0.93
	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 323 and name CB)	16.82	0.94	0.94
25	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 324 and name CA)	18.78	1.17	1.17
	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 324 and name CB)	18.71	1.12	1.13
	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 382 and name CA)	18.55	0.37	0.36
	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 382 and name CB)	18.67	0.43	0.43
	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 383 and name CA)	18.42	0.32	0.33
30	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 384 and name CA)	14.75	0.29	0.28
	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 384 and name CB)	14.39	0.28	0.29
	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 385 and name CA)	14.03	0.33	0.33
	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 386 and name CA)	13.47	0.18	0.18
	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 387 and name CA)	11.49	0.15	0.14
35	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 388 and name C)	7.16	0.13	0.13
	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 388 and name CA)	8.00	0.19	0.20
	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 388 and name CB)	7.90	0.30	0.30
	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 388 and name O)	6.01	0.16	0.17
	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 389 and name CA)	7.64	0.23	0.24
40	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 389 and name CB)	8.48	0.24	0.24
	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 390 and name CA)	9.55	0.37	0.37
	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 390 and name CB)	10.03	0.43	0.43
	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 391 and name CA)	9.91	0.35	0.36
	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 391 and name CB)	11.38	0.36	0.36
45	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 392 and name CA)	7.98	0.26	0.25
	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 392 and name CB)	6.93	0.22	0.21
	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 393 and name CA)	11.43	0.25	0.24
	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 394 and name CA)	13.51	0.28	0.28
50	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 394 and name CB)	13.24	0.27	0.28
	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 395 and name CA)	15.03	0.32	0.32
	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 396 and name CA)	15.98	0.28	0.29
	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 396 and name CB)	15.23	0.34	0.33
	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 397 and name CA)	17.34	0.36	0.36
	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 397 and name CB)	16.71	0.40	0.40
55	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 398 and name CB)	19.10	0.33	0.32
	assign (segid 3A4 and resid 79 and name CB) (segid HEM and resid 1 and name CBD)	6.59	0.38	0.37
	assign (segid 3A4 and resid 79 and name CB) (segid HEM and resid 1 and name CGD)	5.90	0.36	0.37
	assign (segid 3A4 and resid 79 and name CB) (segid HEM and resid 1 and name OLD)	5.14	0.62	0.62
	assign (segid 3A4 and resid 79 and name CB) (segid HEM and resid 1 and name O2D)	6.39	0.61	0.61
60	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 79 and name CG)	1.52	0.01	0.01
	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 80 and name C)	5.45	0.10	0.10
	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 80 and name CA)	4.50	0.08	0.08
	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 80 and name N)	3.17	0.09	0.09
	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 80 and name O)	6.32	0.18	0.18
65	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 81 and name C)	7.00	0.12	0.12
	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 81 and name CA)	6.84	0.08	0.08
	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 81 and name CB)	7.30	0.12	0.12
	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 81 and name N)	5.63	0.08	0.08
	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 82 and name C)	6.89	0.15	0.15
70	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 82 and name CA)	6.72	0.28	0.28
	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 82 and name CB)	6.33	0.53	0.54
	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 82 and name N)	6.14	0.18	0.19
	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 83 and name CA)	6.61	0.12	0.11
	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 83 and name CB)	5.95	0.16	0.17
75	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 83 and name N)	6.07	0.07	0.08
	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 84 and name CA)	9.86	0.23	0.23
	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 84 and name CB)	10.28	0.36	0.36
	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 85 and name CA)	11.51	0.17	0.17
	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 85 and name CB)	11.50	0.22	0.23
80	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 86 and name CA)	10.98	0.20	0.21
	assign (segid 3A4 and resid 79 and name CB) (segid 3A4 and resid 86 and name CB)	10.08	0.39	0.38
	assign (segid 3A4 and resid 79 and name CG) (segid 3A4 and resid 388 and name C)	6.45	0.26	0.26

	assign (segid 3A4 and resid 79 and name CG) (segid 3A4 and resid 388 and name CA)	7.30	0.39	0.38
	assign (segid 3A4 and resid 79 and name CG) (segid 3A4 and resid 388 and name CB)	7.42	0.54	0.54
	assign (segid 3A4 and resid 79 and name CG) (segid 3A4 and resid 388 and name O)	5.27	0.25	0.25
	assign (segid 3A4 and resid 79 and name CG) (segid 3A4 and resid 389 and name CA)	7.00	0.28	0.29
5	assign (segid 3A4 and resid 79 and name CG) (segid 3A4 and resid 389 and name N)	7.24	0.24	0.24
	assign (segid 3A4 and resid 79 and name CG) (segid 3A4 and resid 390 and name O)	6.73	0.47	0.47
	assign (segid 3A4 and resid 79 and name CG) (segid 3A4 and resid 392 and name CA)	6.84	0.45	0.45
	assign (segid 3A4 and resid 79 and name CG) (segid 3A4 and resid 392 and name CB)	5.95	0.42	0.42
	assign (segid 3A4 and resid 79 and name CG) (segid HEM and resid 1 and name CBD)	6.10	0.47	0.47
10	assign (segid 3A4 and resid 79 and name CG) (segid HEM and resid 1 and name CGD)	5.62	0.39	0.39
	assign (segid 3A4 and resid 79 and name CG) (segid HEM and resid 1 and name O1D)	4.87	0.73	0.73
	assign (segid 3A4 and resid 79 and name CG) (segid HEM and resid 1 and name O2D)	6.24	0.64	0.63
	assign (segid 3A4 and resid 79 and name CG) (segid 3A4 and resid 80 and name C)	5.80	0.14	0.14
	assign (segid 3A4 and resid 79 and name CG) (segid 3A4 and resid 80 and name CA)	4.84	0.14	0.15
	assign (segid 3A4 and resid 79 and name CG) (segid 3A4 and resid 80 and name N)	3.79	0.13	0.14
15	assign (segid 3A4 and resid 79 and name CG) (segid 3A4 and resid 80 and name O)	6.44	0.23	0.22
	assign (segid 3A4 and resid 79 and name CG) (segid 3A4 and resid 81 and name C)	7.34	0.12	0.12
	assign (segid 3A4 and resid 79 and name CG) (segid 3A4 and resid 81 and name CA)	7.40	0.13	0.13
	assign (segid 3A4 and resid 79 and name CG) (segid 3A4 and resid 81 and name N)	6.23	0.13	0.13
	assign (segid 3A4 and resid 79 and name CG) (segid 3A4 and resid 82 and name C)	6.63	0.16	0.17
20	assign (segid 3A4 and resid 79 and name CG) (segid 3A4 and resid 82 and name CA)	6.78	0.23	0.24
	assign (segid 3A4 and resid 79 and name CG) (segid 3A4 and resid 82 and name CB)	6.42	0.45	0.45
	assign (segid 3A4 and resid 79 and name CG) (segid 3A4 and resid 82 and name N)	6.43	0.17	0.18
	assign (segid 3A4 and resid 79 and name CG) (segid 3A4 and resid 82 and name O)	7.61	0.18	0.18
25	assign (segid 3A4 and resid 79 and name CG) (segid 3A4 and resid 83 and name C)	7.36	0.22	0.22
	assign (segid 3A4 and resid 79 and name CG) (segid 3A4 and resid 83 and name CA)	5.93	0.23	0.22
	assign (segid 3A4 and resid 79 and name CG) (segid 3A4 and resid 83 and name CB)	5.17	0.21	0.22
	assign (segid 3A4 and resid 79 and name CG) (segid 3A4 and resid 83 and name N)	5.69	0.14	0.14
	assign (segid 3A4 and resid 79 and name CG) (segid HEM and resid 1 and name CGD)	7.33	0.39	0.39
30	assign (segid 3A4 and resid 79 and name N) (segid HEM and resid 1 and name O1D)	6.67	0.51	0.51
	assign (segid 3A4 and resid 79 and name N) (segid 3A4 and resid 79 and name C)	2.46	0.03	0.03
	assign (segid 3A4 and resid 79 and name N) (segid 3A4 and resid 79 and name CA)	1.46	0.01	0.02
	assign (segid 3A4 and resid 79 and name N) (segid 3A4 and resid 79 and name CB)	2.45	0.03	0.02
	assign (segid 3A4 and resid 79 and name N) (segid 3A4 and resid 79 and name CG)	3.82	0.03	0.03
35	assign (segid 3A4 and resid 79 and name N) (segid 3A4 and resid 79 and name O)	3.50	0.06	0.07
	assign (segid 3A4 and resid 79 and name N) (segid 3A4 and resid 80 and name C)	4.75	0.07	0.07
	assign (segid 3A4 and resid 79 and name N) (segid 3A4 and resid 80 and name CA)	4.21	0.06	0.06
	assign (segid 3A4 and resid 79 and name N) (segid 3A4 and resid 80 and name N)	2.82	0.06	0.05
	assign (segid 3A4 and resid 79 and name N) (segid 3A4 and resid 80 and name O)	5.85	0.14	0.13
40	assign (segid 3A4 and resid 79 and name N) (segid 3A4 and resid 81 and name C)	5.83	0.20	0.20
	assign (segid 3A4 and resid 79 and name N) (segid 3A4 and resid 81 and name CA)	5.42	0.07	0.06
	assign (segid 3A4 and resid 79 and name N) (segid 3A4 and resid 81 and name CB)	5.46	0.08	0.08
	assign (segid 3A4 and resid 79 and name N) (segid 3A4 and resid 81 and name N)	4.37	0.05	0.05
	assign (segid 3A4 and resid 79 and name N) (segid 3A4 and resid 81 and name O)	7.04	0.21	0.21
45	assign (segid 3A4 and resid 79 and name N) (segid 3A4 and resid 82 and name C)	6.67	0.36	0.35
	assign (segid 3A4 and resid 79 and name N) (segid 3A4 and resid 82 and name CA)	6.00	0.46	0.47
	assign (segid 3A4 and resid 79 and name N) (segid 3A4 and resid 82 and name CB)	5.66	0.69	0.69
	assign (segid 3A4 and resid 79 and name N) (segid 3A4 and resid 82 and name N)	5.12	0.35	0.35
	assign (segid 3A4 and resid 79 and name N) (segid 3A4 and resid 83 and name CA)	7.12	0.15	0.15
50	assign (segid 3A4 and resid 79 and name N) (segid 3A4 and resid 83 and name CB)	6.77	0.11	0.12
	assign (segid 3A4 and resid 79 and name N) (segid 3A4 and resid 83 and name N)	6.16	0.24	0.24
	assign (segid 3A4 and resid 79 and name N) (segid 3A4 and resid 83 and name O)	6.60	0.42	0.42
	assign (segid 3A4 and resid 79 and name O) (segid 3A4 and resid 79 and name CB)	3.38	0.07	0.07
	assign (segid 3A4 and resid 79 and name O) (segid 3A4 and resid 79 and name CG)	3.40	0.12	0.12
55	assign (segid 3A4 and resid 79 and name O) (segid 3A4 and resid 80 and name C)	2.91	0.11	0.10
	assign (segid 3A4 and resid 79 and name O) (segid 3A4 and resid 80 and name CA)	2.77	0.01	0.02
	assign (segid 3A4 and resid 79 and name O) (segid 3A4 and resid 80 and name N)	2.25	0.00	0.00
	assign (segid 3A4 and resid 79 and name O) (segid 3A4 and resid 80 and name O)	3.43	0.25	0.24
	assign (segid 3A4 and resid 79 and name O) (segid 3A4 and resid 81 and name C)	4.00	0.17	0.16
60	assign (segid 3A4 and resid 79 and name O) (segid 3A4 and resid 81 and name CA)	4.21	0.14	0.14
	assign (segid 3A4 and resid 79 and name O) (segid 3A4 and resid 81 and name CB)	5.14	0.18	0.19
	assign (segid 3A4 and resid 79 and name O) (segid 3A4 and resid 81 and name N)	3.27	0.13	0.14
	assign (segid 3A4 and resid 79 and name O) (segid 3A4 and resid 81 and name O)	4.97	0.17	0.17
	assign (segid 3A4 and resid 79 and name O) (segid 3A4 and resid 82 and name C)	3.80	0.14	0.15
65	assign (segid 3A4 and resid 79 and name O) (segid 3A4 and resid 82 and name CA)	3.82	0.25	0.25
	assign (segid 3A4 and resid 79 and name O) (segid 3A4 and resid 82 and name CB)	4.04	0.40	0.40
	assign (segid 3A4 and resid 79 and name O) (segid 3A4 and resid 82 and name N)	3.22	0.22	0.22
	assign (segid 3A4 and resid 79 and name O) (segid 3A4 and resid 82 and name O)	4.96	0.12	0.13
	assign (segid 3A4 and resid 79 and name O) (segid 3A4 and resid 83 and name C)	5.01	0.12	0.12
70	assign (segid 3A4 and resid 79 and name O) (segid 3A4 and resid 83 and name CA)	3.71	0.08	0.08
	assign (segid 3A4 and resid 79 and name O) (segid 3A4 and resid 83 and name CB)	3.38	0.15	0.16
	assign (segid 3A4 and resid 79 and name O) (segid 3A4 and resid 83 and name N)	2.92	0.09	0.09
	assign (segid 3A4 and resid 79 and name O) (segid 3A4 and resid 83 and name O)	6.04	0.08	0.08
	assign (segid 3A4 and resid 79 and name O) (segid 3A4 and resid 84 and name CA)	6.68	0.34	0.33
75	assign (segid 3A4 and resid 79 and name O) (segid 3A4 and resid 84 and name CB)	7.07	0.39	0.39
	assign (segid 3A4 and resid 79 and name O) (segid 3A4 and resid 84 and name N)	5.27	0.29	0.30
	assign (segid 3A4 and resid 79 and name O) (segid 3A4 and resid 85 and name N)	7.29	0.31	0.31
	assign (segid 3A4 and resid 7 and name C) (segid 3A4 and resid 10 and name C)	4.87	0.06	0.07
80	assign (segid 3A4 and resid 7 and name C) (segid 3A4 and resid 10 and name CA)	4.61	0.07	0.07
	assign (segid 3A4 and resid 7 and name C) (segid 3A4 and resid 10 and name CB)	4.48	0.10	0.11
	assign (segid 3A4 and resid 7 and name C) (segid 3A4 and resid 10 and name N)	3.87	0.10	0.10
	assign (segid 3A4 and resid 7 and name C) (segid 3A4 and resid 10 and name O)	6.06	0.06	0.06
	assign (segid 3A4 and resid 7 and name C) (segid 3A4 and resid 11 and name C)	6.13	0.06	0.07

	assign (segid 3A4 and resid 7 and name C) (segid 3A4 and resid 11 and name CA)	5.02	0.08	0.08
	assign (segid 3A4 and resid 7 and name C) (segid 3A4 and resid 11 and name CB)	4.58	0.11	0.11
	assign (segid 3A4 and resid 7 and name C) (segid 3A4 and resid 11 and name N)	4.14	0.07	0.07
	assign (segid 3A4 and resid 7 and name C) (segid 3A4 and resid 11 and name O)	7.26	0.07	0.07
	assign (segid 3A4 and resid 7 and name C) (segid 3A4 and resid 12 and name CA)	7.41	0.16	0.16
5	assign (segid 3A4 and resid 7 and name C) (segid 3A4 and resid 12 and name N)	6.10	0.14	0.13
	assign (segid 3A4 and resid 7 and name C) (segid 3A4 and resid 7 and name CB)	2.49	0.02	0.03
	assign (segid 3A4 and resid 7 and name C) (segid 3A4 and resid 7 and name O)	1.23	0.01	0.00
	assign (segid 3A4 and resid 7 and name C) (segid 3A4 and resid 8 and name C)	3.08	0.03	0.04
	assign (segid 3A4 and resid 7 and name C) (segid 3A4 and resid 8 and name CA)	2.45	0.02	0.03
10	assign (segid 3A4 and resid 7 and name C) (segid 3A4 and resid 8 and name CB)	3.71	0.03	0.02
	assign (segid 3A4 and resid 7 and name C) (segid 3A4 and resid 8 and name N)	1.34	0.02	0.01
	assign (segid 3A4 and resid 7 and name C) (segid 3A4 and resid 8 and name O)	3.95	0.07	0.07
	assign (segid 3A4 and resid 7 and name C) (segid 3A4 and resid 9 and name C)	4.58	0.09	0.09
	assign (segid 3A4 and resid 7 and name C) (segid 3A4 and resid 9 and name CA)	4.50	0.07	0.06
15	assign (segid 3A4 and resid 7 and name C) (segid 3A4 and resid 9 and name CB)	5.27	0.11	0.11
	assign (segid 3A4 and resid 7 and name C) (segid 3A4 and resid 9 and name N)	3.32	0.06	0.06
	assign (segid 3A4 and resid 7 and name C) (segid 3A4 and resid 9 and name O)	5.66	0.11	0.10
	assign (segid 3A4 and resid 7 and name CA) (segid 3A4 and resid 10 and name C)	5.67	0.11	0.10
	assign (segid 3A4 and resid 7 and name CA) (segid 3A4 and resid 10 and name CA)	5.15	0.17	0.16
20	assign (segid 3A4 and resid 7 and name CA) (segid 3A4 and resid 10 and name CB)	4.59	0.22	0.23
	assign (segid 3A4 and resid 7 and name CA) (segid 3A4 and resid 10 and name N)	4.56	0.16	0.16
	assign (segid 3A4 and resid 7 and name CA) (segid 3A4 and resid 10 and name O)	6.82	0.14	0.13
	assign (segid 3A4 and resid 7 and name CA) (segid 3A4 and resid 11 and name C)	7.37	0.05	0.06
	assign (segid 3A4 and resid 7 and name CA) (segid 3A4 and resid 11 and name CA)	6.15	0.05	0.05
25	assign (segid 3A4 and resid 7 and name CA) (segid 3A4 and resid 11 and name CB)	5.82	0.10	0.11
	assign (segid 3A4 and resid 7 and name CA) (segid 3A4 and resid 11 and name N)	5.17	0.06	0.05
	assign (segid 3A4 and resid 7 and name CA) (segid 3A4 and resid 12 and name CA)	8.73	0.14	0.14
	assign (segid 3A4 and resid 7 and name CA) (segid 3A4 and resid 12 and name CB)	8.89	0.27	0.27
	assign (segid 3A4 and resid 7 and name CA) (segid 3A4 and resid 12 and name N)	7.40	0.12	0.12
30	assign (segid 3A4 and resid 7 and name CA) (segid 3A4 and resid 13 and name CA)	9.99	0.25	0.25
	assign (segid 3A4 and resid 7 and name CA) (segid 3A4 and resid 13 and name CB)	9.55	0.30	0.30
	assign (segid 3A4 and resid 7 and name CA) (segid 3A4 and resid 19 and name CA)	14.06	1.62	1.63
	assign (segid 3A4 and resid 7 and name CA) (segid 3A4 and resid 19 and name CB)	15.11	1.57	1.56
	assign (segid 3A4 and resid 7 and name CA) (segid 3A4 and resid 20 and name CA)	15.24	1.49	1.49
35	assign (segid 3A4 and resid 7 and name CA) (segid 3A4 and resid 20 and name CB)	16.55	1.41	1.42
	assign (segid 3A4 and resid 7 and name CA) (segid 3A4 and resid 21 and name CA)	15.04	1.84	1.84
	assign (segid 3A4 and resid 7 and name CA) (segid 3A4 and resid 21 and name CB)	14.13	1.91	1.92
	assign (segid 3A4 and resid 7 and name CA) (segid 3A4 and resid 22 and name CA)	16.18	2.11	2.11
	assign (segid 3A4 and resid 7 and name CA) (segid 3A4 and resid 23 and name CA)	14.76	2.09	2.10
40	assign (segid 3A4 and resid 7 and name CA) (segid 3A4 and resid 23 and name CB)	13.45	2.03	2.02
	assign (segid 3A4 and resid 7 and name CA) (segid 3A4 and resid 25 and name CA)	16.78	1.67	1.67
	assign (segid 3A4 and resid 7 and name CA) (segid 3A4 and resid 314 and name CA)	14.06	1.95	1.95
	assign (segid 3A4 and resid 7 and name CA) (segid 3A4 and resid 314 and name CB)	14.84	1.96	1.97
45	assign (segid 3A4 and resid 7 and name CA) (segid 3A4 and resid 315 and name CA)	12.20	2.31	2.31
	assign (segid 3A4 and resid 7 and name CA) (segid 3A4 and resid 315 and name CB)	13.10	2.41	2.41
	assign (segid 3A4 and resid 7 and name CA) (segid 3A4 and resid 316 and name CA)	11.38	2.46	2.46
	assign (segid 3A4 and resid 7 and name CA) (segid 3A4 and resid 317 and name CA)	11.23	1.89	1.88
	assign (segid 3A4 and resid 7 and name CA) (segid 3A4 and resid 318 and name CA)	12.36	2.35	2.34
50	assign (segid 3A4 and resid 7 and name CA) (segid 3A4 and resid 318 and name CB)	13.60	2.52	2.53
	assign (segid 3A4 and resid 7 and name CA) (segid 3A4 and resid 319 and name CA)	12.63	2.27	2.28
	assign (segid 3A4 and resid 7 and name CA) (segid 3A4 and resid 319 and name CB)	13.84	2.30	2.29
	assign (segid 3A4 and resid 7 and name CA) (segid 3A4 and resid 31 and name CA)	15.96	1.72	1.73
	assign (segid 3A4 and resid 7 and name CA) (segid 3A4 and resid 31 and name CB)	17.03	1.58	1.59
	assign (segid 3A4 and resid 7 and name CA) (segid 3A4 and resid 322 and name CA)	16.79	2.03	2.03
55	assign (segid 3A4 and resid 7 and name CA) (segid 3A4 and resid 32 and name CA)	12.65	1.52	1.52
	assign (segid 3A4 and resid 7 and name CA) (segid 3A4 and resid 32 and name CB)	11.46	1.58	1.58
	assign (segid 3A4 and resid 7 and name CA) (segid 3A4 and resid 33 and name CA)	13.22	1.14	1.15
	assign (segid 3A4 and resid 7 and name CA) (segid 3A4 and resid 33 and name CB)	14.24	1.02	1.03
60	assign (segid 3A4 and resid 7 and name CA) (segid 3A4 and resid 343 and name CA)	17.07	1.78	1.78
	assign (segid 3A4 and resid 7 and name CA) (segid 3A4 and resid 343 and name CB)	17.72	1.67	1.67
	assign (segid 3A4 and resid 7 and name CA) (segid 3A4 and resid 344 and name CA)	13.81	1.82	1.82
	assign (segid 3A4 and resid 7 and name CA) (segid 3A4 and resid 344 and name CB)	12.90	1.87	1.87
	assign (segid 3A4 and resid 7 and name CA) (segid 3A4 and resid 345 and name CA)	13.07	1.62	1.62
65	assign (segid 3A4 and resid 7 and name CA) (segid 3A4 and resid 345 and name CB)	14.24	1.61	1.61
	assign (segid 3A4 and resid 7 and name CA) (segid 3A4 and resid 346 and name CA)	9.86	1.42	1.42
	assign (segid 3A4 and resid 7 and name CA) (segid 3A4 and resid 346 and name CB)	8.91	1.15	1.16
	assign (segid 3A4 and resid 7 and name CA) (segid 3A4 and resid 347 and name CA)	11.20	1.22	1.22
	assign (segid 3A4 and resid 7 and name CA) (segid 3A4 and resid 347 and name CB)	11.99	1.47	1.47
70	assign (segid 3A4 and resid 7 and name CA) (segid 3A4 and resid 348 and name CA)	8.61	1.15	1.14
	assign (segid 3A4 and resid 7 and name CA) (segid 3A4 and resid 349 and name CA)	8.30	0.94	0.95
	assign (segid 3A4 and resid 7 and name CA) (segid 3A4 and resid 349 and name CB)	8.28	0.74	0.73
	assign (segid 3A4 and resid 7 and name CA) (segid 3A4 and resid 34 and name CA)	11.05	1.00	0.99
	assign (segid 3A4 and resid 7 and name CA) (segid 3A4 and resid 34 and name CB)	10.43	1.31	1.32
75	assign (segid 3A4 and resid 7 and name CA) (segid 3A4 and resid 350 and name CA)	11.61	0.82	0.82
	assign (segid 3A4 and resid 7 and name CA) (segid 3A4 and resid 350 and name CB)	12.49	0.62	0.62
	assign (segid 3A4 and resid 7 and name CA) (segid 3A4 and resid 351 and name CA)	11.93	1.33	1.33
	assign (segid 3A4 and resid 7 and name CA) (segid 3A4 and resid 352 and name CA)	10.37	1.99	1.98
	assign (segid 3A4 and resid 7 and name CA) (segid 3A4 and resid 352 and name CB)	9.05	2.17	2.11
	assign (segid 3A4 and resid 7 and name CA) (segid 3A4 and resid 353 and name CA)	12.49	1.79	1.79
80	assign (segid 3A4 and resid 7 and name CA) (segid 3A4 and resid 353 and name CB)	13.26	1.64	1.63
	assign (segid 3A4 and resid 7 and name CA) (segid 3A4 and resid 354 and name CA)	14.71	2.09	2.08
	assign (segid 3A4 and resid 7 and name CA) (segid 3A4 and resid 354 and name CB)	14.71	2.16	2.16

	assign (segid 3A4 and resid 7 and name CA)	(segid 3A4 and resid 357 and name CB)	15.68	2.13	2.13
	assign (segid 3A4 and resid 7 and name CA)	(segid 3A4 and resid 35 and name CA)	13.51	1.02	1.01
	assign (segid 3A4 and resid 7 and name CA)	(segid 3A4 and resid 360 and name CA)	13.26	2.57	2.57
	assign (segid 3A4 and resid 7 and name CA)	(segid 3A4 and resid 360 and name CB)	12.53	2.49	2.50
5	assign (segid 3A4 and resid 7 and name CA)	(segid 3A4 and resid 361 and name CA)	11.92	2.77	2.77
	assign (segid 3A4 and resid 7 and name CA)	(segid 3A4 and resid 361 and name CB)	11.46	2.83	2.83
	assign (segid 3A4 and resid 7 and name CA)	(segid 3A4 and resid 36 and name CA)	15.13	1.20	1.20
	assign (segid 3A4 and resid 7 and name CA)	(segid 3A4 and resid 381 and name CA)	16.63	1.67	1.68
	assign (segid 3A4 and resid 7 and name CA)	(segid 3A4 and resid 382 and name CA)	15.95	1.09	1.09
10	assign (segid 3A4 and resid 7 and name CA)	(segid 3A4 and resid 382 and name CB)	15.52	0.85	0.84
	assign (segid 3A4 and resid 7 and name CA)	(segid 3A4 and resid 383 and name CA)	15.13	1.54	1.54
	assign (segid 3A4 and resid 7 and name CA)	(segid 3A4 and resid 38 and name CA)	17.52	0.94	0.94
	assign (segid 3A4 and resid 7 and name CA)	(segid 3A4 and resid 38 and name CB)	16.75	1.08	1.09
	assign (segid 3A4 and resid 7 and name CA)	(segid 3A4 and resid 39 and name CA)	16.17	0.77	0.77
	assign (segid 3A4 and resid 7 and name CA)	(segid 3A4 and resid 39 and name CB)	14.99	0.76	0.77
15	assign (segid 3A4 and resid 7 and name CA)	(segid 3A4 and resid 426 and name CA)	14.03	2.05	2.05
	assign (segid 3A4 and resid 7 and name CA)	(segid 3A4 and resid 427 and name CA)	13.27	2.65	2.65
	assign (segid 3A4 and resid 7 and name CA)	(segid 3A4 and resid 428 and name CA)	12.47	2.20	2.20
	assign (segid 3A4 and resid 7 and name CA)	(segid 3A4 and resid 429 and name CA)	11.73	2.01	2.02
20	assign (segid 3A4 and resid 7 and name CA)	(segid 3A4 and resid 430 and name CA)	11.62	0.93	0.94
	assign (segid 3A4 and resid 7 and name CA)	(segid 3A4 and resid 431 and name CA)	12.96	1.96	1.95
	assign (segid 3A4 and resid 7 and name CA)	(segid 3A4 and resid 433 and name CA)	11.77	2.01	2.00
	assign (segid 3A4 and resid 7 and name CA)	(segid 3A4 and resid 434 and name CA)	13.94	2.15	2.15
	assign (segid 3A4 and resid 7 and name CA)	(segid 3A4 and resid 7 and name C)	1.52	0.02	0.01
25	assign (segid 3A4 and resid 7 and name CA)	(segid 3A4 and resid 7 and name CB)	1.53	0.02	0.02
	assign (segid 3A4 and resid 7 and name CA)	(segid 3A4 and resid 7 and name O)	2.39	0.04	0.04
	assign (segid 3A4 and resid 7 and name CA)	(segid 3A4 and resid 8 and name C)	4.45	0.03	0.03
	assign (segid 3A4 and resid 7 and name CA)	(segid 3A4 and resid 8 and name CA)	3.82	0.02	0.03
	assign (segid 3A4 and resid 7 and name CA)	(segid 3A4 and resid 8 and name CB)	4.86	0.02	0.02
30	assign (segid 3A4 and resid 7 and name CA)	(segid 3A4 and resid 8 and name N)	2.45	0.03	0.03
	assign (segid 3A4 and resid 7 and name CA)	(segid 3A4 and resid 8 and name O)	5.40	0.06	0.06
	assign (segid 3A4 and resid 7 and name CA)	(segid 3A4 and resid 9 and name C)	5.48	0.13	0.12
	assign (segid 3A4 and resid 7 and name CA)	(segid 3A4 and resid 9 and name CA)	5.45	0.08	0.08
	assign (segid 3A4 and resid 7 and name CA)	(segid 3A4 and resid 9 and name CB)	5.91	0.15	0.15
	assign (segid 3A4 and resid 7 and name CA)	(segid 3A4 and resid 9 and name N)	4.39	0.07	0.07
35	assign (segid 3A4 and resid 7 and name CA)	(segid 3A4 and resid 9 and name O)	6.61	0.13	0.13
	assign (segid 3A4 and resid 7 and name CA)	(segid 3A4 and resid 10 and name C)	6.71	0.07	0.06
	assign (segid 3A4 and resid 7 and name CB)	(segid 3A4 and resid 10 and name CA)	6.38	0.12	0.12
	assign (segid 3A4 and resid 7 and name CB)	(segid 3A4 and resid 10 and name CB)	5.71	0.21	0.20
40	assign (segid 3A4 and resid 7 and name CB)	(segid 3A4 and resid 10 and name N)	5.94	0.12	0.13
	assign (segid 3A4 and resid 7 and name CB)	(segid 3A4 and resid 10 and name O)	7.79	0.09	0.09
	assign (segid 3A4 and resid 7 and name CB)	(segid 3A4 and resid 11 and name CA)	6.82	0.16	0.15
	assign (segid 3A4 and resid 7 and name CB)	(segid 3A4 and resid 11 and name CB)	6.25	0.23	0.22
	assign (segid 3A4 and resid 7 and name CB)	(segid 3A4 and resid 11 and name N)	6.07	0.11	0.11
45	assign (segid 3A4 and resid 7 and name CB)	(segid 3A4 and resid 12 and name CA)	9.72	0.23	0.22
	assign (segid 3A4 and resid 7 and name CB)	(segid 3A4 and resid 12 and name CB)	9.99	0.33	0.34
	assign (segid 3A4 and resid 7 and name CB)	(segid 3A4 and resid 13 and name CA)	11.10	0.14	0.13
	assign (segid 3A4 and resid 7 and name CB)	(segid 3A4 and resid 13 and name CB)	10.72	0.17	0.17
	assign (segid 3A4 and resid 7 and name CB)	(segid 3A4 and resid 19 and name CA)	14.58	1.70	1.70
50	assign (segid 3A4 and resid 7 and name CB)	(segid 3A4 and resid 19 and name CB)	15.55	1.58	1.58
	assign (segid 3A4 and resid 7 and name CB)	(segid 3A4 and resid 20 and name CA)	15.81	1.77	1.77
	assign (segid 3A4 and resid 7 and name CB)	(segid 3A4 and resid 21 and name CA)	15.78	2.29	2.28
	assign (segid 3A4 and resid 7 and name CB)	(segid 3A4 and resid 21 and name CB)	14.92	2.36	2.37
	assign (segid 3A4 and resid 7 and name CB)	(segid 3A4 and resid 23 and name CA)	15.59	2.69	2.70
55	assign (segid 3A4 and resid 7 and name CB)	(segid 3A4 and resid 23 and name CB)	14.27	2.60	2.60
	assign (segid 3A4 and resid 7 and name CB)	(segid 3A4 and resid 314 and name CA)	13.15	2.38	2.37
	assign (segid 3A4 and resid 7 and name CB)	(segid 3A4 and resid 314 and name CB)	13.94	2.40	2.40
	assign (segid 3A4 and resid 7 and name CB)	(segid 3A4 and resid 315 and name CA)	11.24	2.78	2.78
	assign (segid 3A4 and resid 7 and name CB)	(segid 3A4 and resid 315 and name CB)	12.12	2.89	2.90
60	assign (segid 3A4 and resid 7 and name CB)	(segid 3A4 and resid 316 and name CA)	10.45	2.83	2.83
	assign (segid 3A4 and resid 7 and name CB)	(segid 3A4 and resid 317 and name CA)	10.39	2.21	2.21
	assign (segid 3A4 and resid 7 and name CB)	(segid 3A4 and resid 318 and name CA)	11.65	2.53	2.53
	assign (segid 3A4 and resid 7 and name CB)	(segid 3A4 and resid 318 and name CB)	12.88	2.70	2.69
	assign (segid 3A4 and resid 7 and name CB)	(segid 3A4 and resid 319 and name CA)	12.08	2.59	2.59
65	assign (segid 3A4 and resid 7 and name CB)	(segid 3A4 and resid 319 and name CB)	13.28	2.60	2.59
	assign (segid 3A4 and resid 7 and name CB)	(segid 3A4 and resid 31 and name CA)	16.54	2.11	2.12
	assign (segid 3A4 and resid 7 and name CB)	(segid 3A4 and resid 32 and name CA)	13.17	1.88	1.88
	assign (segid 3A4 and resid 7 and name CB)	(segid 3A4 and resid 32 and name CB)	12.05	1.97	1.97
	assign (segid 3A4 and resid 7 and name CB)	(segid 3A4 and resid 33 and name CA)	13.56	1.40	1.40
70	assign (segid 3A4 and resid 7 and name CB)	(segid 3A4 and resid 33 and name CB)	14.49	1.26	1.27
	assign (segid 3A4 and resid 7 and name CB)	(segid 3A4 and resid 344 and name CA)	14.06	2.10	2.10
	assign (segid 3A4 and resid 7 and name CB)	(segid 3A4 and resid 344 and name CB)	13.23	2.14	2.14
	assign (segid 3A4 and resid 7 and name CB)	(segid 3A4 and resid 345 and name CA)	13.12	1.88	1.89
	assign (segid 3A4 and resid 7 and name CB)	(segid 3A4 and resid 345 and name CB)	14.21	1.90	1.89
75	assign (segid 3A4 and resid 7 and name CB)	(segid 3A4 and resid 346 and name CA)	9.88	1.67	1.67
	assign (segid 3A4 and resid 7 and name CB)	(segid 3A4 and resid 346 and name CB)	9.08	1.38	1.39
	assign (segid 3A4 and resid 7 and name CB)	(segid 3A4 and resid 347 and name CA)	10.85	1.54	1.53
	assign (segid 3A4 and resid 7 and name CB)	(segid 3A4 and resid 347 and name CB)	11.55	1.82	1.82
	assign (segid 3A4 and resid 7 and name CB)	(segid 3A4 and resid 348 and name CA)	8.18	1.40	1.39
80	assign (segid 3A4 and resid 7 and name CB)	(segid 3A4 and resid 349 and name CA)	8.25	0.88	0.88
	assign (segid 3A4 and resid 7 and name CB)	(segid 3A4 and resid 349 and name CB)	8.41	0.60	0.60
	assign (segid 3A4 and resid 7 and name CB)	(segid 3A4 and resid 34 and name CA)	11.37	1.02	1.03
	assign (segid 3A4 and resid 7 and name CB)	(segid 3A4 and resid 34 and name CB)	10.89	1.35	1.34

	assign (segid 3A4 and resid 7 and name CB) (segid 3A4 and resid 350 and name CA)	11.34	0.86	0.86
	assign (segid 3A4 and resid 7 and name CB) (segid 3A4 and resid 350 and name CB)	12.18	0.72	0.73
	assign (segid 3A4 and resid 7 and name CB) (segid 3A4 and resid 351 and name CA)	11.33	1.58	1.59
	assign (segid 3A4 and resid 7 and name CB) (segid 3A4 and resid 352 and name CA)	9.93	2.20	2.19
	assign (segid 3A4 and resid 7 and name CB) (segid 3A4 and resid 352 and name CB)	8.64	2.34	2.33
5	assign (segid 3A4 and resid 7 and name CB) (segid 3A4 and resid 353 and name CA)	12.30	1.81	1.82
	assign (segid 3A4 and resid 7 and name CB) (segid 3A4 and resid 353 and name CB)	13.08	1.61	1.61
	assign (segid 3A4 and resid 7 and name CB) (segid 3A4 and resid 354 and name CA)	14.52	2.15	2.15
	assign (segid 3A4 and resid 7 and name CB) (segid 3A4 and resid 354 and name CB)	14.61	2.19	2.19
	assign (segid 3A4 and resid 7 and name CB) (segid 3A4 and resid 357 and name CB)	15.07	2.41	2.42
10	assign (segid 3A4 and resid 7 and name CB) (segid 3A4 and resid 35 and name CA)	13.66	0.88	0.88
	assign (segid 3A4 and resid 7 and name CB) (segid 3A4 and resid 360 and name CA)	12.67	2.93	2.93
	assign (segid 3A4 and resid 7 and name CB) (segid 3A4 and resid 360 and name CB)	12.04	2.80	2.80
	assign (segid 3A4 and resid 7 and name CB) (segid 3A4 and resid 361 and name CA)	11.28	3.21	3.21
	assign (segid 3A4 and resid 7 and name CB) (segid 3A4 and resid 361 and name CB)	10.92	3.23	3.24
15	assign (segid 3A4 and resid 7 and name CB) (segid 3A4 and resid 362 and name CA)	14.63	3.18	3.17
	assign (segid 3A4 and resid 7 and name CB) (segid 3A4 and resid 36 and name CA)	15.00	1.14	1.13
	assign (segid 3A4 and resid 7 and name CB) (segid 3A4 and resid 382 and name CA)	15.32	1.35	1.35
	assign (segid 3A4 and resid 7 and name CB) (segid 3A4 and resid 382 and name CB)	14.98	1.08	1.08
20	assign (segid 3A4 and resid 7 and name CB) (segid 3A4 and resid 383 and name CA)	14.38	1.85	1.85
	assign (segid 3A4 and resid 7 and name CB) (segid 3A4 and resid 38 and name CA)	17.62	0.94	0.94
	assign (segid 3A4 and resid 7 and name CB) (segid 3A4 and resid 38 and name CB)	16.94	1.11	1.12
	assign (segid 3A4 and resid 7 and name CB) (segid 3A4 and resid 39 and name CA)	16.13	0.83	0.83
	assign (segid 3A4 and resid 7 and name CB) (segid 3A4 and resid 39 and name CB)	14.91	0.83	0.83
25	assign (segid 3A4 and resid 7 and name CB) (segid 3A4 and resid 426 and name CA)	13.83	2.14	2.13
	assign (segid 3A4 and resid 7 and name CB) (segid 3A4 and resid 427 and name CA)	13.12	2.61	2.61
	assign (segid 3A4 and resid 7 and name CB) (segid 3A4 and resid 428 and name CA)	12.46	2.26	2.26
	assign (segid 3A4 and resid 7 and name CB) (segid 3A4 and resid 429 and name CA)	11.80	2.14	2.13
	assign (segid 3A4 and resid 7 and name CB) (segid 3A4 and resid 430 and name CA)	11.67	1.25	1.24
30	assign (segid 3A4 and resid 7 and name CB) (segid 3A4 and resid 431 and name CA)	12.79	2.31	2.30
	assign (segid 3A4 and resid 7 and name CB) (segid 3A4 and resid 433 and name CA)	11.37	2.22	2.22
	assign (segid 3A4 and resid 7 and name CB) (segid 3A4 and resid 434 and name CA)	13.44	2.21	2.20
	assign (segid 3A4 and resid 7 and name CB) (segid 3A4 and resid 8 and name C)	5.51	0.07	0.07
	assign (segid 3A4 and resid 7 and name CB) (segid 3A4 and resid 8 and name CA)	4.57	0.09	0.09
35	assign (segid 3A4 and resid 7 and name CB) (segid 3A4 and resid 8 and name CB)	5.46	0.08	0.07
	assign (segid 3A4 and resid 7 and name CB) (segid 3A4 and resid 8 and name N)	3.26	0.08	0.08
	assign (segid 3A4 and resid 7 and name CB) (segid 3A4 and resid 8 and name O)	6.38	0.11	0.11
	assign (segid 3A4 and resid 7 and name CB) (segid 3A4 and resid 9 and name C)	6.87	0.10	0.10
	assign (segid 3A4 and resid 7 and name CB) (segid 3A4 and resid 9 and name CA)	6.85	0.07	0.06
40	assign (segid 3A4 and resid 7 and name CB) (segid 3A4 and resid 9 and name CB)	7.38	0.13	0.14
	assign (segid 3A4 and resid 7 and name CB) (segid 3A4 and resid 9 and name N)	5.68	0.06	0.07
	assign (segid 3A4 and resid 7 and name CB) (segid 3A4 and resid 10 and name C)	6.51	0.18	0.17
	assign (segid 3A4 and resid 7 and name N) (segid 3A4 and resid 10 and name CA)	5.72	0.24	0.25
	assign (segid 3A4 and resid 7 and name N) (segid 3A4 and resid 10 and name CB)	5.24	0.27	0.27
	assign (segid 3A4 and resid 7 and name N) (segid 3A4 and resid 10 and name N)	4.91	0.24	0.24
45	assign (segid 3A4 and resid 7 and name N) (segid 3A4 and resid 11 and name CA)	7.24	0.06	0.06
	assign (segid 3A4 and resid 7 and name N) (segid 3A4 and resid 11 and name CB)	6.98	0.07	0.08
	assign (segid 3A4 and resid 7 and name N) (segid 3A4 and resid 11 and name N)	6.14	0.10	0.09
	assign (segid 3A4 and resid 7 and name N) (segid 3A4 and resid 7 and name C)	2.46	0.05	0.06
50	assign (segid 3A4 and resid 7 and name N) (segid 3A4 and resid 7 and name CA)	1.45	0.01	0.01
	assign (segid 3A4 and resid 7 and name N) (segid 3A4 and resid 7 and name CB)	2.48	0.04	0.04
	assign (segid 3A4 and resid 7 and name N) (segid 3A4 and resid 7 and name O)	3.52	0.08	0.08
	assign (segid 3A4 and resid 7 and name N) (segid 3A4 and resid 8 and name C)	4.77	0.12	0.12
	assign (segid 3A4 and resid 7 and name N) (segid 3A4 and resid 8 and name CA)	4.22	0.08	0.09
	assign (segid 3A4 and resid 7 and name N) (segid 3A4 and resid 8 and name CB)	4.94	0.08	0.08
55	assign (segid 3A4 and resid 7 and name N) (segid 3A4 and resid 8 and name N)	2.81	0.09	0.09
	assign (segid 3A4 and resid 7 and name N) (segid 3A4 and resid 8 and name O)	5.88	0.09	0.10
	assign (segid 3A4 and resid 7 and name N) (segid 3A4 and resid 9 and name C)	5.70	0.24	0.24
	assign (segid 3A4 and resid 7 and name N) (segid 3A4 and resid 9 and name CA)	5.40	0.21	0.21
	assign (segid 3A4 and resid 7 and name N) (segid 3A4 and resid 9 and name CB)	5.52	0.25	0.24
60	assign (segid 3A4 and resid 7 and name N) (segid 3A4 and resid 9 and name N)	4.38	0.17	0.18
	assign (segid 3A4 and resid 7 and name N) (segid 3A4 and resid 9 and name O)	6.90	0.23	0.23
	assign (segid 3A4 and resid 7 and name O) (segid 3A4 and resid 10 and name C)	3.89	0.20	0.21
	assign (segid 3A4 and resid 7 and name O) (segid 3A4 and resid 10 and name CA)	3.90	0.22	0.23
	assign (segid 3A4 and resid 7 and name O) (segid 3A4 and resid 10 and name CB)	3.87	0.16	0.15
65	assign (segid 3A4 and resid 7 and name O) (segid 3A4 and resid 10 and name N)	3.42	0.24	0.25
	assign (segid 3A4 and resid 7 and name O) (segid 3A4 and resid 10 and name O)	5.04	0.18	0.17
	assign (segid 3A4 and resid 7 and name O) (segid 3A4 and resid 11 and name C)	5.09	0.12	0.12
	assign (segid 3A4 and resid 7 and name O) (segid 3A4 and resid 11 and name CA)	3.89	0.11	0.11
	assign (segid 3A4 and resid 7 and name O) (segid 3A4 and resid 11 and name CB)	3.54	0.11	0.12
70	assign (segid 3A4 and resid 7 and name O) (segid 3A4 and resid 11 and name N)	3.06	0.17	0.18
	assign (segid 3A4 and resid 7 and name O) (segid 3A4 and resid 11 and name O)	6.19	0.11	0.11
	assign (segid 3A4 and resid 7 and name O) (segid 3A4 and resid 12 and name C)	7.42	0.17	0.18
	assign (segid 3A4 and resid 7 and name O) (segid 3A4 and resid 12 and name CA)	6.59	0.18	0.18
	assign (segid 3A4 and resid 7 and name O) (segid 3A4 and resid 12 and name CB)	6.94	0.28	0.27
75	assign (segid 3A4 and resid 7 and name O) (segid 3A4 and resid 12 and name N)	5.21	0.17	0.16
	assign (segid 3A4 and resid 7 and name O) (segid 3A4 and resid 13 and name N)	7.10	0.20	0.19
	assign (segid 3A4 and resid 7 and name O) (segid 3A4 and resid 7 and name CB)	3.20	0.08	0.07
	assign (segid 3A4 and resid 7 and name O) (segid 3A4 and resid 8 and name C)	3.06	0.11	0.11
80	assign (segid 3A4 and resid 7 and name O) (segid 3A4 and resid 8 and name CA)	2.77	0.03	0.03
	assign (segid 3A4 and resid 7 and name O) (segid 3A4 and resid 8 and name CB)	4.24	0.02	0.02
	assign (segid 3A4 and resid 7 and name O) (segid 3A4 and resid 8 and name N)	2.24	0.01	0.01
	assign (segid 3A4 and resid 7 and name O) (segid 3A4 and resid 8 and name O)	3.59	0.14	0.14

	assign (segid 3A4 and resid 7 and name O) (segid 3A4 and resid 9 and name C) 4.20 0.24 0.24
	assign (segid 3A4 and resid 7 and name O) (segid 3A4 and resid 9 and name CA) 4.45 0.20 0.20
	assign (segid 3A4 and resid 7 and name O) (segid 3A4 and resid 9 and name CB) 5.44 0.24 0.25
	assign (segid 3A4 and resid 7 and name O) (segid 3A4 and resid 9 and name N) 3.48 0.16 0.16
5	assign (segid 3A4 and resid 7 and name O) (segid 3A4 and resid 9 and name O) 5.12 0.25 0.26
	assign (segid 3A4 and resid 80 and name C) (segid 3A4 and resid 80 and name O) 1.24 0.01 0.00
	assign (segid 3A4 and resid 80 and name C) (segid 3A4 and resid 81 and name C) 3.06 0.05 0.04
	assign (segid 3A4 and resid 80 and name C) (segid 3A4 and resid 81 and name CA) 2.43 0.01 0.01
10	assign (segid 3A4 and resid 80 and name C) (segid 3A4 and resid 81 and name CB) 3.71 0.02 0.01
	assign (segid 3A4 and resid 80 and name C) (segid 3A4 and resid 81 and name N) 1.33 0.00 0.00
	assign (segid 3A4 and resid 80 and name C) (segid 3A4 and resid 81 and name O) 3.91 0.07 0.07
	assign (segid 3A4 and resid 80 and name C) (segid 3A4 and resid 82 and name C) 4.72 0.13 0.13
	assign (segid 3A4 and resid 80 and name C) (segid 3A4 and resid 82 and name CA) 4.55 0.12 0.12
15	assign (segid 3A4 and resid 80 and name C) (segid 3A4 and resid 82 and name CB) 5.46 0.19 0.19
	assign (segid 3A4 and resid 80 and name C) (segid 3A4 and resid 82 and name N) 3.33 0.10 0.11
	assign (segid 3A4 and resid 80 and name C) (segid 3A4 and resid 82 and name O) 5.82 0.16 0.15
	assign (segid 3A4 and resid 80 and name C) (segid 3A4 and resid 83 and name C) 5.44 0.34 0.34
	assign (segid 3A4 and resid 80 and name C) (segid 3A4 and resid 83 and name CA) 4.79 0.16 0.16
	assign (segid 3A4 and resid 80 and name C) (segid 3A4 and resid 83 and name CB) 4.42 0.13 0.13
20	assign (segid 3A4 and resid 80 and name C) (segid 3A4 and resid 83 and name N) 4.01 0.12 0.12
	assign (segid 3A4 and resid 80 and name C) (segid 3A4 and resid 83 and name O) 6.62 0.34 0.35
	assign (segid 3A4 and resid 80 and name C) (segid 3A4 and resid 84 and name CA) 6.11 0.67 0.66
	assign (segid 3A4 and resid 80 and name C) (segid 3A4 and resid 84 and name CB) 5.91 0.74 0.74
	assign (segid 3A4 and resid 80 and name C) (segid 3A4 and resid 84 and name N) 5.02 0.53 0.53
25	assign (segid 3A4 and resid 80 and name CA) (segid 3A4 and resid 137 and name CA) 17.31 0.70 0.70
	assign (segid 3A4 and resid 80 and name CA) (segid 3A4 and resid 138 and name CA) 17.93 1.14 1.13
	assign (segid 3A4 and resid 80 and name CA) (segid 3A4 and resid 202 and name CB) 19.00 0.52 0.53
	assign (segid 3A4 and resid 80 and name CA) (segid 3A4 and resid 219 and name CA) 16.54 0.84 0.84
30	assign (segid 3A4 and resid 80 and name CA) (segid 3A4 and resid 219 and name CB) 17.56 0.71 0.72
	assign (segid 3A4 and resid 80 and name CA) (segid 3A4 and resid 220 and name CA) 13.34 0.65 0.66
	assign (segid 3A4 and resid 80 and name CA) (segid 3A4 and resid 220 and name CB) 13.07 0.62 0.62
	assign (segid 3A4 and resid 80 and name CA) (segid 3A4 and resid 221 and name CA) 14.85 0.31 0.32
	assign (segid 3A4 and resid 80 and name CA) (segid 3A4 and resid 221 and name CB) 16.24 0.30 0.30
35	assign (segid 3A4 and resid 80 and name CA) (segid 3A4 and resid 222 and name CA) 15.74 0.42 0.43
	assign (segid 3A4 and resid 80 and name CA) (segid 3A4 and resid 222 and name CB) 16.66 0.50 0.50
	assign (segid 3A4 and resid 80 and name CA) (segid 3A4 and resid 223 and name CA) 12.38 0.58 0.59
	assign (segid 3A4 and resid 80 and name CA) (segid 3A4 and resid 223 and name CB) 11.63 0.71 0.71
	assign (segid 3A4 and resid 80 and name CA) (segid 3A4 and resid 224 and name CA) 11.08 0.29 0.30
40	assign (segid 3A4 and resid 80 and name CA) (segid 3A4 and resid 224 and name CB) 11.20 0.34 0.34
	assign (segid 3A4 and resid 80 and name CA) (segid 3A4 and resid 225 and name CA) 14.34 0.40 0.41
	assign (segid 3A4 and resid 80 and name CA) (segid 3A4 and resid 225 and name CB) 15.67 0.33 0.33
	assign (segid 3A4 and resid 80 and name CA) (segid 3A4 and resid 226 and name CA) 14.24 0.54 0.53
	assign (segid 3A4 and resid 80 and name CA) (segid 3A4 and resid 240 and name CA) 15.22 0.61 0.62
45	assign (segid 3A4 and resid 80 and name CA) (segid 3A4 and resid 240 and name CB) 15.80 0.68 0.68
	assign (segid 3A4 and resid 80 and name CA) (segid 3A4 and resid 241 and name CA) 17.15 0.26 0.27
	assign (segid 3A4 and resid 80 and name CA) (segid 3A4 and resid 241 and name CB) 18.61 0.29 0.28
	assign (segid 3A4 and resid 80 and name CA) (segid 3A4 and resid 242 and name CA) 17.33 0.32 0.32
	assign (segid 3A4 and resid 80 and name CA) (segid 3A4 and resid 242 and name CB) 18.00 0.44 0.45
50	assign (segid 3A4 and resid 80 and name CA) (segid 3A4 and resid 243 and name CA) 13.68 0.34 0.35
	assign (segid 3A4 and resid 80 and name CA) (segid 3A4 and resid 243 and name CB) 12.73 0.43 0.42
	assign (segid 3A4 and resid 80 and name CA) (segid 3A4 and resid 244 and name CA) 13.40 0.12 0.11
	assign (segid 3A4 and resid 80 and name CA) (segid 3A4 and resid 244 and name CB) 14.02 0.10 0.10
	assign (segid 3A4 and resid 80 and name CA) (segid 3A4 and resid 245 and name CA) 16.43 0.24 0.23
55	assign (segid 3A4 and resid 80 and name CA) (segid 3A4 and resid 245 and name CB) 17.74 0.18 0.18
	assign (segid 3A4 and resid 80 and name CA) (segid 3A4 and resid 246 and name CA) 15.32 0.31 0.31
	assign (segid 3A4 and resid 80 and name CA) (segid 3A4 and resid 246 and name CB) 15.14 0.22 0.23
	assign (segid 3A4 and resid 80 and name CA) (segid 3A4 and resid 247 and name CA) 12.22 0.46 0.47
	assign (segid 3A4 and resid 80 and name CA) (segid 3A4 and resid 247 and name CB) 11.04 0.48 0.47
60	assign (segid 3A4 and resid 80 and name CA) (segid 3A4 and resid 248 and name CA) 14.70 0.66 0.66
	assign (segid 3A4 and resid 80 and name CA) (segid 3A4 and resid 248 and name CB) 15.56 0.64 0.65
	assign (segid 3A4 and resid 80 and name CA) (segid 3A4 and resid 249 and name CA) 17.17 0.63 0.63
	assign (segid 3A4 and resid 80 and name CA) (segid 3A4 and resid 250 and name CA) 15.13 0.64 0.65
	assign (segid 3A4 and resid 80 and name CA) (segid 3A4 and resid 250 and name CB) 13.96 0.65 0.65
65	assign (segid 3A4 and resid 80 and name CA) (segid 3A4 and resid 251 and name CA) 14.34 0.76 0.76
	assign (segid 3A4 and resid 80 and name CA) (segid 3A4 and resid 251 and name CB) 13.66 0.83 0.83
	assign (segid 3A4 and resid 80 and name CA) (segid 3A4 and resid 252 and name CA) 18.07 0.76 0.77
	assign (segid 3A4 and resid 80 and name CA) (segid 3A4 and resid 254 and name CA) 17.45 0.63 0.64
	assign (segid 3A4 and resid 80 and name CA) (segid 3A4 and resid 255 and name CA) 18.14 0.60 0.59
70	assign (segid 3A4 and resid 80 and name CA) (segid 3A4 and resid 384 and name CA) 17.89 0.48 0.49
	assign (segid 3A4 and resid 80 and name CA) (segid 3A4 and resid 384 and name CB) 17.25 0.54 0.54
	assign (segid 3A4 and resid 80 and name CA) (segid 3A4 and resid 385 and name CA) 17.62 0.33 0.34
	assign (segid 3A4 and resid 80 and name CA) (segid 3A4 and resid 386 and name CA) 16.78 0.39 0.39
	assign (segid 3A4 and resid 80 and name CA) (segid 3A4 and resid 387 and name CA) 14.65 0.33 0.33
	assign (segid 3A4 and resid 80 and name CA) (segid 3A4 and resid 388 and name CA) 11.22 0.37 0.37
75	assign (segid 3A4 and resid 80 and name CA) (segid 3A4 and resid 388 and name CB) 11.06 0.46 0.47
	assign (segid 3A4 and resid 80 and name CA) (segid 3A4 and resid 389 and name CA) 11.69 0.33 0.34
	assign (segid 3A4 and resid 80 and name CA) (segid 3A4 and resid 389 and name CB) 12.71 0.31 0.31
	assign (segid 3A4 and resid 80 and name CA) (segid 3A4 and resid 390 and name CA) 12.93 0.47 0.48
80	assign (segid 3A4 and resid 80 and name CA) (segid 3A4 and resid 390 and name CB) 13.04 0.51 0.52
	assign (segid 3A4 and resid 80 and name CA) (segid 3A4 and resid 391 and name CA) 13.02 0.54 0.53
	assign (segid 3A4 and resid 80 and name CA) (segid 3A4 and resid 391 and name CB) 14.36 0.56 0.57
	assign (segid 3A4 and resid 80 and name CA) (segid 3A4 and resid 392 and name CA) 10.17 0.51 0.51
	assign (segid 3A4 and resid 80 and name CA) (segid 3A4 and resid 392 and name CB) 9.17 0.48 0.49

	assign (segid 3A4 and resid 80 and name CA) (segid 3A4 and resid 393 and name CA)	13.14	0.54	0.55
	assign (segid 3A4 and resid 80 and name CA) (segid 3A4 and resid 394 and name CA)	15.31	0.60	0.59
	assign (segid 3A4 and resid 80 and name CA) (segid 3A4 and resid 394 and name CB)	15.12	0.61	0.60
	assign (segid 3A4 and resid 80 and name CA) (segid 3A4 and resid 395 and name CA)	15.77	0.68	0.69
	assign (segid 3A4 and resid 80 and name CA) (segid 3A4 and resid 396 and name CA)	16.71	0.62	0.62
5	assign (segid 3A4 and resid 80 and name CA) (segid 3A4 and resid 396 and name CB)	15.94	0.61	0.62
	assign (segid 3A4 and resid 80 and name CA) (segid 3A4 and resid 397 and name CB)	18.59	0.67	0.67
	assign (segid 3A4 and resid 80 and name CA) (segid 3A4 and resid 80 and name C)	1.52	0.01	0.01
	assign (segid 3A4 and resid 80 and name CA) (segid 3A4 and resid 80 and name O)	2.39	0.02	0.01
	assign (segid 3A4 and resid 80 and name CA) (segid 3A4 and resid 81 and name C)	4.45	0.04	0.03
10	assign (segid 3A4 and resid 80 and name CA) (segid 3A4 and resid 81 and name CA)	3.80	0.01	0.02
	assign (segid 3A4 and resid 80 and name CA) (segid 3A4 and resid 81 and name CB)	4.85	0.02	0.01
	assign (segid 3A4 and resid 80 and name CA) (segid 3A4 and resid 81 and name N)	2.42	0.01	0.02
	assign (segid 3A4 and resid 80 and name CA) (segid 3A4 and resid 81 and name O)	5.36	0.07	0.08
	assign (segid 3A4 and resid 80 and name CA) (segid 3A4 and resid 82 and name C)	5.61	0.09	0.10
15	assign (segid 3A4 and resid 80 and name CA) (segid 3A4 and resid 82 and name CA)	5.57	0.11	0.10
	assign (segid 3A4 and resid 80 and name CA) (segid 3A4 and resid 82 and name CB)	6.23	0.23	0.23
	assign (segid 3A4 and resid 80 and name CA) (segid 3A4 and resid 82 and name N)	4.44	0.09	0.09
	assign (segid 3A4 and resid 80 and name CA) (segid 3A4 and resid 82 and name O)	6.74	0.10	0.10
20	assign (segid 3A4 and resid 80 and name CA) (segid 3A4 and resid 83 and name C)	6.08	0.23	0.22
	assign (segid 3A4 and resid 80 and name CA) (segid 3A4 and resid 83 and name CA)	5.23	0.16	0.16
	assign (segid 3A4 and resid 80 and name CA) (segid 3A4 and resid 83 and name CB)	4.47	0.21	0.21
	assign (segid 3A4 and resid 80 and name CA) (segid 3A4 and resid 83 and name N)	4.67	0.11	0.11
	assign (segid 3A4 and resid 80 and name CA) (segid 3A4 and resid 83 and name O)	7.19	0.24	0.25
25	assign (segid 3A4 and resid 80 and name CA) (segid 3A4 and resid 84 and name C)	7.04	0.50	0.50
	assign (segid 3A4 and resid 80 and name CA) (segid 3A4 and resid 84 and name CB)	6.96	0.59	0.58
	assign (segid 3A4 and resid 80 and name CA) (segid 3A4 and resid 84 and name N)	5.89	0.38	0.37
	assign (segid 3A4 and resid 80 and name CA) (segid 3A4 and resid 85 and name CA)	9.52	0.37	0.38
	assign (segid 3A4 and resid 80 and name CA) (segid 3A4 and resid 85 and name CB)	9.65	0.38	0.38
	assign (segid 3A4 and resid 80 and name CA) (segid 3A4 and resid 85 and name N)	10.31	0.26	0.25
30	assign (segid 3A4 and resid 80 and name CA) (segid 3A4 and resid 86 and name CA)	9.95	0.34	0.35
	assign (segid 3A4 and resid 80 and name CA) (segid 3A4 and resid 86 and name CB)	18.03	0.93	0.92
	assign (segid 3A4 and resid 80 and name CA) (segid 3A4 and resid 86 and name N)	2.47	0.03	0.02
	assign (segid 3A4 and resid 80 and name CA) (segid 3A4 and resid 86 and name O)	1.45	0.01	0.01
35	assign (segid 3A4 and resid 80 and name N) (segid 3A4 and resid 80 and name C)	3.50	0.07	0.06
	assign (segid 3A4 and resid 80 and name N) (segid 3A4 and resid 80 and name O)	4.78	0.06	0.05
	assign (segid 3A4 and resid 80 and name N) (segid 3A4 and resid 81 and name C)	4.23	0.02	0.02
	assign (segid 3A4 and resid 80 and name N) (segid 3A4 and resid 81 and name CB)	4.97	0.05	0.06
	assign (segid 3A4 and resid 80 and name N) (segid 3A4 and resid 81 and name N)	2.82	0.04	0.04
40	assign (segid 3A4 and resid 80 and name N) (segid 3A4 and resid 81 and name O)	5.87	0.08	0.08
	assign (segid 3A4 and resid 80 and name N) (segid 3A4 and resid 82 and name C)	5.73	0.09	0.09
	assign (segid 3A4 and resid 80 and name N) (segid 3A4 and resid 82 and name CA)	5.51	0.16	0.15
	assign (segid 3A4 and resid 80 and name N) (segid 3A4 and resid 82 and name CB)	5.82	0.35	0.36
	assign (segid 3A4 and resid 80 and name N) (segid 3A4 and resid 82 and name N)	1.44	0.11	0.11
45	assign (segid 3A4 and resid 80 and name N) (segid 3A4 and resid 82 and name O)	6.92	0.08	0.09
	assign (segid 3A4 and resid 80 and name N) (segid 3A4 and resid 83 and name C)	6.66	0.15	0.15
	assign (segid 3A4 and resid 80 and name N) (segid 3A4 and resid 83 and name CA)	5.55	0.08	0.09
	assign (segid 3A4 and resid 80 and name N) (segid 3A4 and resid 83 and name CB)	4.87	0.16	0.16
	assign (segid 3A4 and resid 80 and name N) (segid 3A4 and resid 83 and name N)	4.85	0.05	0.06
50	assign (segid 3A4 and resid 80 and name N) (segid 3A4 and resid 84 and name N)	6.66	0.35	0.35
	assign (segid 3A4 and resid 80 and name O) (segid 3A4 and resid 81 and name C)	3.02	0.09	0.08
	assign (segid 3A4 and resid 80 and name O) (segid 3A4 and resid 81 and name CA)	2.77	0.03	0.04
	assign (segid 3A4 and resid 80 and name O) (segid 3A4 and resid 81 and name CB)	4.26	0.05	0.05
	assign (segid 3A4 and resid 80 and name O) (segid 3A4 and resid 81 and name N)	2.26	0.02	0.02
55	assign (segid 3A4 and resid 80 and name O) (segid 3A4 and resid 81 and name O)	3.52	0.10	0.09
	assign (segid 3A4 and resid 80 and name O) (segid 3A4 and resid 82 and name C)	4.35	0.28	0.28
	assign (segid 3A4 and resid 80 and name O) (segid 3A4 and resid 82 and name CA)	4.47	0.23	0.23
	assign (segid 3A4 and resid 80 and name O) (segid 3A4 and resid 82 and name CB)	5.61	0.28	0.27
	assign (segid 3A4 and resid 80 and name O) (segid 3A4 and resid 82 and name N)	3.48	0.19	0.19
60	assign (segid 3A4 and resid 80 and name O) (segid 3A4 and resid 82 and name O)	5.31	0.32	0.31
	assign (segid 3A4 and resid 80 and name O) (segid 3A4 and resid 83 and name C)	4.60	0.53	0.52
	assign (segid 3A4 and resid 80 and name O) (segid 3A4 and resid 83 and name CA)	4.21	0.34	0.35
	assign (segid 3A4 and resid 80 and name O) (segid 3A4 and resid 83 and name CB)	3.92	0.26	0.26
	assign (segid 3A4 and resid 80 and name O) (segid 3A4 and resid 83 and name N)	3.62	0.27	0.28
65	assign (segid 3A4 and resid 80 and name O) (segid 3A4 and resid 83 and name O)	5.78	0.56	0.55
	assign (segid 3A4 and resid 80 and name O) (segid 3A4 and resid 84 and name C)	6.24	0.70	0.71
	assign (segid 3A4 and resid 80 and name O) (segid 3A4 and resid 84 and name CA)	5.05	0.75	0.74
	assign (segid 3A4 and resid 80 and name O) (segid 3A4 and resid 84 and name CB)	4.84	0.72	0.71
	assign (segid 3A4 and resid 80 and name O) (segid 3A4 and resid 84 and name N)	4.03	0.64	0.64
70	assign (segid 3A4 and resid 80 and name O) (segid 3A4 and resid 85 and name N)	6.27	0.65	0.66
	assign (segid 3A4 and resid 81 and name C) (segid 3A4 and resid 81 and name CB)	2.51	0.02	0.03
	assign (segid 3A4 and resid 81 and name C) (segid 3A4 and resid 81 and name O)	1.24	0.01	0.01
	assign (segid 3A4 and resid 81 and name C) (segid 3A4 and resid 82 and name C)	3.23	0.17	0.18
	assign (segid 3A4 and resid 81 and name C) (segid 3A4 and resid 82 and name CA)	2.44	0.02	0.02
75	assign (segid 3A4 and resid 81 and name C) (segid 3A4 and resid 82 and name CB)	3.65	0.06	0.06
	assign (segid 3A4 and resid 81 and name C) (segid 3A4 and resid 82 and name N)	1.33	0.00	0.00
	assign (segid 3A4 and resid 81 and name C) (segid 3A4 and resid 82 and name O)	4.13	0.25	0.25
	assign (segid 3A4 and resid 81 and name C) (segid 3A4 and resid 83 and name C)	5.14	0.45	0.45
	assign (segid 3A4 and resid 81 and name C) (segid 3A4 and resid 83 and name CA)	4.76	0.24	0.24
80	assign (segid 3A4 and resid 81 and name C) (segid 3A4 and resid 83 and name CB)	5.33	0.16	0.17
	assign (segid 3A4 and resid 81 and name C) (segid 3A4 and resid 83 and name N)	3.49	0.18	0.18
	assign (segid 3A4 and resid 81 and name C) (segid 3A4 and resid 83 and name O)	6.28	0.44	0.44
	assign (segid 3A4 and resid 81 and name C) (segid 3A4 and resid 84 and name C)	6.09	0.81	0.81

5	assign (segid 3A4 and resid 81 and name C) (segid 3A4 and resid 84 and name CA) 5.50 0.79 0.80
	assign (segid 3A4 and resid 81 and name C) (segid 3A4 and resid 84 and name CB) 5.33 0.90 0.89
	assign (segid 3A4 and resid 81 and name C) (segid 3A4 and resid 84 and name N) 4.57 0.65 0.65
	assign (segid 3A4 and resid 81 and name C) (segid 3A4 and resid 85 and name CB) 6.08 0.78 0.78
	assign (segid 3A4 and resid 81 and name C) (segid 3A4 and resid 85 and name N) 5.52 0.80 0.80
10	assign (segid 3A4 and resid 81 and name CA) (segid 3A4 and resid 134 and name CA) 17.94 0.90 0.91
	assign (segid 3A4 and resid 81 and name CA) (segid 3A4 and resid 137 and name CA) 14.91 0.86 0.86
	assign (segid 3A4 and resid 81 and name CA) (segid 3A4 and resid 138 and name CA) 15.10 1.00 0.99
	assign (segid 3A4 and resid 81 and name CA) (segid 3A4 and resid 138 and name CB) 15.58 1.04 1.05
	assign (segid 3A4 and resid 81 and name CA) (segid 3A4 and resid 139 and name CA) 17.64 0.92 0.92
15	assign (segid 3A4 and resid 81 and name CA) (segid 3A4 and resid 198 and name CA) 18.45 0.68 0.67
	assign (segid 3A4 and resid 81 and name CA) (segid 3A4 and resid 198 and name CB) 17.53 0.71 0.70
	assign (segid 3A4 and resid 81 and name CA) (segid 3A4 and resid 201 and name CB) 18.32 0.71 0.72
	assign (segid 3A4 and resid 81 and name CA) (segid 3A4 and resid 202 and name CA) 16.20 0.77 0.76
	assign (segid 3A4 and resid 81 and name CA) (segid 3A4 and resid 202 and name CB) 15.63 0.66 0.67
20	assign (segid 3A4 and resid 81 and name CA) (segid 3A4 and resid 205 and name CA) 17.17 0.96 0.97
	assign (segid 3A4 and resid 81 and name CA) (segid 3A4 and resid 205 and name CB) 15.99 0.94 0.94
	assign (segid 3A4 and resid 81 and name CA) (segid 3A4 and resid 206 and name CA) 17.00 0.94 0.95
	assign (segid 3A4 and resid 81 and name CA) (segid 3A4 and resid 206 and name CB) 17.11 0.92 0.92
	assign (segid 3A4 and resid 81 and name CA) (segid 3A4 and resid 219 and name CA) 13.47 0.89 0.88
25	assign (segid 3A4 and resid 81 and name CA) (segid 3A4 and resid 219 and name CB) 14.44 0.75 0.75
	assign (segid 3A4 and resid 81 and name CA) (segid 3A4 and resid 220 and name CA) 10.29 0.75 0.75
	assign (segid 3A4 and resid 81 and name CA) (segid 3A4 and resid 220 and name CB) 10.28 0.71 0.70
	assign (segid 3A4 and resid 81 and name CA) (segid 3A4 and resid 221 and name CA) 11.43 0.39 0.38
	assign (segid 3A4 and resid 81 and name CA) (segid 3A4 and resid 221 and name CB) 12.84 0.35 0.36
30	assign (segid 3A4 and resid 81 and name CA) (segid 3A4 and resid 222 and name CA) 12.08 0.47 0.47
	assign (segid 3A4 and resid 81 and name CA) (segid 3A4 and resid 222 and name CB) 13.05 0.54 0.54
	assign (segid 3A4 and resid 81 and name CA) (segid 3A4 and resid 223 and name CA) 8.80 0.65 0.65
	assign (segid 3A4 and resid 81 and name CA) (segid 3A4 and resid 223 and name CB) 8.21 0.80 0.81
	assign (segid 3A4 and resid 81 and name CA) (segid 3A4 and resid 224 and name CA) 7.40 0.34 0.33
35	assign (segid 3A4 and resid 81 and name CA) (segid 3A4 and resid 224 and name CB) 7.67 0.37 0.36
	assign (segid 3A4 and resid 81 and name CA) (segid 3A4 and resid 225 and name CA) 10.63 0.42 0.42
	assign (segid 3A4 and resid 81 and name CA) (segid 3A4 and resid 225 and name CB) 11.94 0.34 0.33
	assign (segid 3A4 and resid 81 and name CA) (segid 3A4 and resid 226 and name CA) 10.62 0.56 0.55
	assign (segid 3A4 and resid 81 and name CA) (segid 3A4 and resid 240 and name CA) 12.70 0.59 0.58
40	assign (segid 3A4 and resid 81 and name CA) (segid 3A4 and resid 240 and name CB) 13.55 0.60 0.60
	assign (segid 3A4 and resid 81 and name CA) (segid 3A4 and resid 241 and name CA) 14.28 0.29 0.29
	assign (segid 3A4 and resid 81 and name CA) (segid 3A4 and resid 241 and name CB) 15.68 0.31 0.31
	assign (segid 3A4 and resid 81 and name CA) (segid 3A4 and resid 242 and name CA) 15.02 0.33 0.34
	assign (segid 3A4 and resid 81 and name CA) (segid 3A4 and resid 242 and name CB) 15.90 0.41 0.41
45	assign (segid 3A4 and resid 81 and name CA) (segid 3A4 and resid 243 and name CA) 11.64 0.42 0.43
	assign (segid 3A4 and resid 81 and name CA) (segid 3A4 and resid 243 and name CB) 10.78 0.45 0.46
	assign (segid 3A4 and resid 81 and name CA) (segid 3A4 and resid 244 and name CA) 10.60 0.30 0.29
	assign (segid 3A4 and resid 81 and name CA) (segid 3A4 and resid 244 and name CB) 10.96 0.29 0.28
	assign (segid 3A4 and resid 81 and name CA) (segid 3A4 and resid 245 and name CA) 13.86 0.38 0.38
50	assign (segid 3A4 and resid 81 and name CA) (segid 3A4 and resid 245 and name CB) 15.19 0.35 0.35
	assign (segid 3A4 and resid 81 and name CA) (segid 3A4 and resid 246 and name CA) 13.52 0.50 0.50
	assign (segid 3A4 and resid 81 and name CA) (segid 3A4 and resid 246 and name CB) 13.57 0.43 0.44
	assign (segid 3A4 and resid 81 and name CA) (segid 3A4 and resid 247 and name CA) 10.39 0.62 0.63
	assign (segid 3A4 and resid 81 and name CA) (segid 3A4 and resid 247 and name CB) 8.99 0.63 0.62
55	assign (segid 3A4 and resid 81 and name CA) (segid 3A4 and resid 248 and name CA) 12.36 0.78 0.79
	assign (segid 3A4 and resid 81 and name CA) (segid 3A4 and resid 248 and name CB) 12.96 0.78 0.78
	assign (segid 3A4 and resid 81 and name CA) (segid 3A4 and resid 249 and name CA) 15.36 0.75 0.75
	assign (segid 3A4 and resid 81 and name CA) (segid 3A4 and resid 250 and name CA) 14.06 0.74 0.74
	assign (segid 3A4 and resid 81 and name CA) (segid 3A4 and resid 250 and name CB) 13.08 0.76 0.75
60	assign (segid 3A4 and resid 81 and name CA) (segid 3A4 and resid 251 and name CA) 13.04 0.82 0.81
	assign (segid 3A4 and resid 81 and name CA) (segid 3A4 and resid 251 and name CB) 12.06 0.88 0.88
	assign (segid 3A4 and resid 81 and name CA) (segid 3A4 and resid 252 and name CA) 16.52 0.83 0.83
	assign (segid 3A4 and resid 81 and name CA) (segid 3A4 and resid 252 and name CB) 17.07 0.86 0.85
	assign (segid 3A4 and resid 81 and name CA) (segid 3A4 and resid 253 and name CA) 18.46 0.78 0.79
65	assign (segid 3A4 and resid 81 and name CA) (segid 3A4 and resid 254 and name CA) 17.08 0.74 0.74
	assign (segid 3A4 and resid 81 and name CA) (segid 3A4 and resid 255 and name CA) 17.49 0.72 0.73
	assign (segid 3A4 and resid 81 and name CA) (segid 3A4 and resid 387 and name CA) 17.78 0.33 0.32
	assign (segid 3A4 and resid 81 and name CA) (segid 3A4 and resid 388 and name CA) 14.40 0.32 0.31
	assign (segid 3A4 and resid 81 and name CA) (segid 3A4 and resid 388 and name CB) 14.31 0.37 0.36
70	assign (segid 3A4 and resid 81 and name CA) (segid 3A4 and resid 389 and name CA) 14.19 0.32 0.32
	assign (segid 3A4 and resid 81 and name CA) (segid 3A4 and resid 389 and name CB) 15.07 0.36 0.36
	assign (segid 3A4 and resid 81

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	assign (segid 3A4 and resid 81 and name CB)	(segid 3A4 and resid 390 and name CB)	16.46	0.41	0.41
	assign (segid 3A4 and resid 81 and name CB)	(segid 3A4 and resid 391 and name CA)	15.25	0.47	0.46
	assign (segid 3A4 and resid 81 and name CB)	(segid 3A4 and resid 391 and name CB)	16.43	0.49	0.49
	assign (segid 3A4 and resid 81 and name CB)	(segid 3A4 and resid 392 and name CA)	12.11	0.47	0.46
	assign (segid 3A4 and resid 81 and name CB)	(segid 3A4 and resid 392 and name CB)	10.77	0.45	0.45
5	assign (segid 3A4 and resid 81 and name CB)	(segid 3A4 and resid 393 and name CA)	14.23	0.56	0.56
	assign (segid 3A4 and resid 81 and name CB)	(segid 3A4 and resid 394 and name CA)	17.22	0.59	0.59
	assign (segid 3A4 and resid 81 and name CB)	(segid 3A4 and resid 394 and name CB)	17.42	0.58	0.59
	assign (segid 3A4 and resid 81 and name CB)	(segid 3A4 and resid 395 and name CA)	17.51	0.76	0.76
	assign (segid 3A4 and resid 81 and name CB)	(segid 3A4 and resid 396 and name CA)	17.43	0.75	0.74
10	assign (segid 3A4 and resid 81 and name CB)	(segid 3A4 and resid 396 and name CB)	16.33	0.74	0.75
	assign (segid 3A4 and resid 81 and name CB)	(segid 3A4 and resid 82 and name C)	5.58	0.11	0.12
	assign (segid 3A4 and resid 81 and name CB)	(segid 3A4 and resid 82 and name CA)	4.49	0.05	0.05
	assign (segid 3A4 and resid 81 and name CB)	(segid 3A4 and resid 82 and name CB)	5.20	0.10	0.10
	assign (segid 3A4 and resid 81 and name CB)	(segid 3A4 and resid 82 and name N)	3.17	0.04	0.05
15	assign (segid 3A4 and resid 81 and name CB)	(segid 3A4 and resid 82 and name O)	6.53	0.21	0.21
	assign (segid 3A4 and resid 81 and name CB)	(segid 3A4 and resid 83 and name CA)	7.03	0.15	0.15
	assign (segid 3A4 and resid 81 and name CB)	(segid 3A4 and resid 83 and name CB)	7.33	0.11	0.11
	assign (segid 3A4 and resid 81 and name CB)	(segid 3A4 and resid 83 and name N)	5.75	0.10	0.11
20	assign (segid 3A4 and resid 81 and name CB)	(segid 3A4 and resid 84 and name CA)	7.74	0.94	0.93
	assign (segid 3A4 and resid 81 and name CB)	(segid 3A4 and resid 84 and name CB)	7.27	1.16	1.17
	assign (segid 3A4 and resid 81 and name CB)	(segid 3A4 and resid 85 and name CA)	8.68	0.98	0.98
	assign (segid 3A4 and resid 81 and name CB)	(segid 3A4 and resid 85 and name CB)	8.07	1.03	1.02
	assign (segid 3A4 and resid 81 and name CB)	(segid 3A4 and resid 86 and name CA)	10.56	0.75	0.75
	assign (segid 3A4 and resid 81 and name CB)	(segid 3A4 and resid 86 and name CB)	10.30	0.63	0.63
25	assign (segid 3A4 and resid 81 and name CB)	(segid 3A4 and resid 94 and name CA)	18.43	0.97	0.97
	assign (segid 3A4 and resid 81 and name CB)	(segid 3A4 and resid 94 and name CB)	17.57	0.90	0.91
	assign (segid 3A4 and resid 81 and name N)	(segid 3A4 and resid 81 and name C)	2.48	0.01	0.01
	assign (segid 3A4 and resid 81 and name N)	(segid 3A4 and resid 81 and name CA)	1.46	0.00	0.00
	assign (segid 3A4 and resid 81 and name N)	(segid 3A4 and resid 81 and name CB)	2.45	0.01	0.01
30	assign (segid 3A4 and resid 81 and name N)	(segid 3A4 and resid 81 and name O)	3.52	0.03	0.03
	assign (segid 3A4 and resid 81 and name N)	(segid 3A4 and resid 82 and name C)	4.84	0.08	0.08
	assign (segid 3A4 and resid 81 and name N)	(segid 3A4 and resid 82 and name CA)	4.26	0.05	0.05
	assign (segid 3A4 and resid 81 and name N)	(segid 3A4 and resid 82 and name CB)	5.08	0.11	0.11
	assign (segid 3A4 and resid 81 and name N)	(segid 3A4 and resid 82 and name N)	2.84	0.05	0.05
35	assign (segid 3A4 and resid 81 and name N)	(segid 3A4 and resid 82 and name O)	5.96	0.12	0.13
	assign (segid 3A4 and resid 81 and name N)	(segid 3A4 and resid 83 and name C)	6.17	0.34	0.33
	assign (segid 3A4 and resid 81 and name N)	(segid 3A4 and resid 83 and name CA)	5.50	0.14	0.13
	assign (segid 3A4 and resid 81 and name N)	(segid 3A4 and resid 83 and name CB)	5.39	0.14	0.14
	assign (segid 3A4 and resid 81 and name N)	(segid 3A4 and resid 83 and name N)	4.44	0.10	0.10
40	assign (segid 3A4 and resid 81 and name N)	(segid 3A4 and resid 83 and name O)	7.36	0.32	0.32
	assign (segid 3A4 and resid 81 and name N)	(segid 3A4 and resid 84 and name CA)	6.74	0.74	0.75
	assign (segid 3A4 and resid 81 and name N)	(segid 3A4 and resid 84 and name CB)	6.46	0.90	0.90
	assign (segid 3A4 and resid 81 and name N)	(segid 3A4 and resid 84 and name N)	5.70	0.58	0.57
	assign (segid 3A4 and resid 81 and name N)	(segid 3A4 and resid 223 and name C)	6.70	0.49	0.50
45	assign (segid 3A4 and resid 81 and name O)	(segid 3A4 and resid 223 and name O)	6.55	0.55	0.55
	assign (segid 3A4 and resid 81 and name O)	(segid 3A4 and resid 224 and name CA)	6.63	0.51	0.51
	assign (segid 3A4 and resid 81 and name O)	(segid 3A4 and resid 224 and name N)	6.74	0.46	0.46
	assign (segid 3A4 and resid 81 and name O)	(segid 3A4 and resid 81 and name CB)	3.29	0.08	0.07
	assign (segid 3A4 and resid 81 and name O)	(segid 3A4 and resid 82 and name C)	3.31	0.27	0.28
50	assign (segid 3A4 and resid 81 and name O)	(segid 3A4 and resid 82 and name CA)	2.77	0.03	0.04
	assign (segid 3A4 and resid 81 and name O)	(segid 3A4 and resid 82 and name CB)	4.16	0.12	0.11
	assign (segid 3A4 and resid 81 and name O)	(segid 3A4 and resid 82 and name N)	2.26	0.02	0.01
	assign (segid 3A4 and resid 81 and name O)	(segid 3A4 and resid 82 and name O)	3.89	0.40	0.40
	assign (segid 3A4 and resid 81 and name O)	(segid 3A4 and resid 83 and name C)	4.93	0.65	0.65
55	assign (segid 3A4 and resid 81 and name O)	(segid 3A4 and resid 83 and name CA)	4.89	0.41	0.41
	assign (segid 3A4 and resid 81 and name O)	(segid 3A4 and resid 83 and name CB)	5.66	0.32	0.31
	assign (segid 3A4 and resid 81 and name O)	(segid 3A4 and resid 83 and name N)	3.79	0.28	0.29
	assign (segid 3A4 and resid 81 and name O)	(segid 3A4 and resid 83 and name O)	5.99	0.68	0.68
	assign (segid 3A4 and resid 81 and name O)	(segid 3A4 and resid 84 and name C)	5.29	1.03	1.04
60	assign (segid 3A4 and resid 81 and name O)	(segid 3A4 and resid 84 and name CA)	4.87	0.98	0.98
	assign (segid 3A4 and resid 81 and name O)	(segid 3A4 and resid 84 and name CB)	4.60	1.03	1.03
	assign (segid 3A4 and resid 81 and name O)	(segid 3A4 and resid 84 and name N)	4.17	0.80	0.81
	assign (segid 3A4 and resid 81 and name O)	(segid 3A4 and resid 85 and name CA)	5.59	1.03	1.04
	assign (segid 3A4 and resid 81 and name O)	(segid 3A4 and resid 85 and name CB)	5.20	0.97	0.97
65	assign (segid 3A4 and resid 81 and name O)	(segid 3A4 and resid 85 and name N)	4.69	1.04	1.03
	assign (segid 3A4 and resid 82 and name C)	(segid 3A4 and resid 392 and name CB)	6.50	0.63	0.62
	assign (segid 3A4 and resid 82 and name C)	(segid 3A4 and resid 82 and name CB)	2.51	0.02	0.01
	assign (segid 3A4 and resid 82 and name C)	(segid 3A4 and resid 82 and name O)	1.23	0.00	0.01
	assign (segid 3A4 and resid 82 and name C)	(segid 3A4 and resid 83 and name C)	3.03	0.06	0.05
70	assign (segid 3A4 and resid 82 and name C)	(segid 3A4 and resid 83 and name CA)	2.45	0.01	0.01
	assign (segid 3A4 and resid 82 and name C)	(segid 3A4 and resid 83 and name CB)	3.70	0.02	0.02
	assign (segid 3A4 and resid 82 and name C)	(segid 3A4 and resid 83 and name N)	1.33	0.01	0.01
	assign (segid 3A4 and resid 82 and name C)	(segid 3A4 and resid 83 and name O)	3.92	0.12	0.11
	assign (segid 3A4 and resid 82 and name C)	(segid 3A4 and resid 84 and name C)	4.68	0.17	0.17
75	assign (segid 3A4 and resid 82 and name C)	(segid 3A4 and resid 84 and name CA)	4.43	0.11	0.11
	assign (segid 3A4 and resid 82 and name C)	(segid 3A4 and resid 84 and name CB)	5.12	0.15	0.16
	assign (segid 3A4 and resid 82 and name C)	(segid 3A4 and resid 84 and name N)	3.23	0.11	0.11
	assign (segid 3A4 and resid 82 and name C)	(segid 3A4 and resid 84 and name O)	5.82	0.23	0.22
	assign (segid 3A4 and resid 82 and name C)	(segid 3A4 and resid 95 and name C)	5.14	0.31	0.32
80	assign (segid 3A4 and resid 82 and name C)	(segid 3A4 and resid 85 and name CA)	4.83	0.26	0.26
	assign (segid 3A4 and resid 82 and name C)	(segid 3A4 and resid 85 and name CB)	4.81	0.34	0.34
	assign (segid 3A4 and resid 82 and name C)	(segid 3A4 and resid 85 and name N)	4.01	0.20	0.20

	assign (segid 3A4 and resid 82 and name C) (segid 3A4 and resid 85 and name O)	6.28	0.33	0.34
	assign (segid 3A4 and resid 82 and name C) (segid 3A4 and resid 86 and name C)	6.12	0.51	0.52
	assign (segid 3A4 and resid 82 and name C) (segid 3A4 and resid 86 and name CA)	5.33	0.43	0.42
	assign (segid 3A4 and resid 82 and name C) (segid 3A4 and resid 86 and name CB)	4.97	0.44	0.45
5	assign (segid 3A4 and resid 82 and name C) (segid 3A4 and resid 86 and name N)	4.46	0.39	0.39
	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 133 and name CA)	15.84	1.42	1.43
	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 133 and name CB)	15.81	1.48	1.49
	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 134 and name CA)	14.65	0.99	1.00
	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 135 and name CA)	15.92	0.78	0.77
10	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 135 and name CB)	17.20	0.84	0.83
	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 136 and name CA)	14.78	1.50	1.50
	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 136 and name CB)	15.03	2.01	2.01
	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 137 and name CA)	12.00	0.72	0.72
	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 138 and name CA)	12.59	1.23	1.23
15	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 138 and name CB)	13.04	1.30	1.29
	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 139 and name CA)	15.37	1.01	1.00
	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 140 and name CA)	17.87	0.90	0.90
	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 140 and name CB)	17.82	1.01	1.02
	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 198 and name CA)	16.91	0.64	0.63
20	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 198 and name CB)	15.94	0.66	0.66
	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 199 and name CA)	18.20	0.50	0.50
	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 201 and name CA)	17.68	0.64	0.63
	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 201 and name CB)	16.85	0.59	0.59
	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 202 and name CA)	15.60	0.62	0.62
25	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 202 and name CB)	15.14	0.55	0.56
	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 205 and name CA)	16.71	0.90	0.91
	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 205 and name CB)	15.37	0.89	0.89
	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 206 and name CA)	17.36	0.86	0.87
	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 206 and name CB)	17.61	0.84	0.83
30	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 219 and name CA)	11.55	0.85	0.84
	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 219 and name CB)	12.45	0.72	0.71
	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 220 and name CA)	8.19	0.64	0.65
	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 220 and name CB)	7.76	0.63	0.63
	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 221 and name CA)	10.06	0.39	0.39
35	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 221 and name CB)	11.38	0.41	0.40
	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 222 and name CA)	11.52	0.49	0.50
	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 222 and name CB)	12.40	0.53	0.54
	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 223 and name CA)	8.62	0.68	0.68
	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 223 and name CB)	7.65	0.81	0.81
40	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 224 and name CA)	7.59	0.64	0.64
	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 224 and name CB)	7.37	0.74	0.73
	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 225 and name CA)	11.28	0.71	0.72
	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 225 and name CB)	12.31	0.61	0.60
	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 226 and name CA)	12.02	0.74	0.74
45	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 240 and name CA)	14.26	0.81	0.80
	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 240 and name CB)	15.12	0.77	0.76
	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 241 and name CA)	15.00	0.49	0.50
	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 241 and name CB)	16.39	0.48	0.47
	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 242 and name CA)	15.36	0.55	0.54
50	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 242 and name CB)	16.39	0.58	0.58
	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 243 and name CA)	12.03	0.57	0.58
	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 243 and name CB)	11.59	0.62	0.63
	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 244 and name CA)	10.46	0.44	0.44
	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 244 and name CB)	11.01	0.43	0.43
55	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 245 and name CA)	13.00	0.48	0.48
	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 245 and name CB)	14.47	0.48	0.48
	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 246 and name CA)	12.45	0.62	0.62
	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 246 and name CB)	12.80	0.53	0.54
	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 247 and name CA)	8.83	0.66	0.65
60	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 247 and name CB)	7.64	0.65	0.66
	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 248 and name CA)	10.21	0.83	0.83
	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 248 and name CB)	11.03	0.84	0.83
	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 249 and name CA)	13.11	0.83	0.83
	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 250 and name CA)	11.55	0.83	0.83
65	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 250 and name CB)	10.76	0.82	0.82
	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 251 and name CA)	9.88	0.87	0.87
	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 251 and name CB)	8.90	0.91	0.90
	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 252 and name CA)	13.38	0.88	0.87
	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 252 and name CB)	14.09	0.88	0.88
70	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 253 and name CA)	15.42	0.91	0.91
	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 254 and name CA)	13.89	0.89	0.89
	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 255 and name CA)	13.99	0.85	0.85
	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 256 and name CA)	17.18	0.74	0.73
	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 258 and name CB)	17.77	1.06	1.06
75	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 259 and name CB)	18.10	0.65	0.65
	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 384 and name CA)	16.86	0.69	0.68
	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 384 and name CB)	16.16	0.73	0.73
	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 385 and name CA)	17.56	0.62	0.63
	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 386 and name CA)	17.82	0.61	0.61
80	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 387 and name CA)	16.69	0.57	0.57
	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 388 and name CA)	13.73	0.56	0.56
	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 388 and name CB)	14.00	0.58	0.58
	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 389 and name CA)	12.81	0.56	0.57

	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 389 and name CB)	13.72	0.63	0.63
	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 390 and name CA)	13.30	0.62	0.63
	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 390 and name CB)	13.68	0.62	0.62
	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 391 and name CA)	11.80	0.68	0.69
5	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 391 and name CB)	12.80	0.70	0.71
	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 392 and name CA)	8.36	0.61	0.62
	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 392 and name CB)	7.12	0.63	0.62
	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 393 and name CA)	10.01	0.65	0.65
	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 394 and name CA)	13.09	0.69	0.68
10	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 394 and name CB)	13.43	0.71	0.72
	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 395 and name CA)	13.29	0.77	0.78
	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 396 and name CA)	13.08	0.71	0.71
	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 396 and name CB)	12.01	0.70	0.69
	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 397 and name CA)	15.48	0.72	0.72
15	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 397 and name CB)	15.39	0.72	0.72
	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 398 and name CA)	17.86	0.74	0.73
	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 398 and name CB)	17.82	0.75	0.74
	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 399 and name CA)	18.00	0.71	0.71
	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 399 and name CB)	16.99	0.71	0.71
20	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 400 and name CA)	18.04	0.70	0.71
	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 82 and name C)	1.53	0.01	0.01
	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 82 and name CB)	1.53	0.01	0.02
	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 82 and name O)	2.40	0.02	0.02
	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 83 and name C)	4.46	0.05	0.06
	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 83 and name CB)	3.83	0.01	0.00
25	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 83 and name CA)	4.85	0.03	0.02
	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 83 and name N)	2.44	0.01	0.02
	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 83 and name O)	5.41	0.12	0.11
	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 84 and name C)	5.77	0.23	0.23
30	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 84 and name CA)	5.54	0.18	0.18
	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 84 and name CB)	5.93	0.30	0.29
	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 84 and name N)	4.43	0.16	0.16
	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 84 and name O)	6.93	0.27	0.28
	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 85 and name C)	6.10	0.43	0.43
35	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 85 and name CA)	5.62	0.34	0.35
	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 85 and name CB)	5.21	0.42	0.42
	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 85 and name N)	4.95	0.25	0.25
	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 86 and name CA)	6.48	0.54	0.54
	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 86 and name CB)	6.03	0.57	0.57
40	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 86 and name N)	5.59	0.50	0.49
	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 94 and name CA)	14.79	0.89	0.89
	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 94 and name CB)	13.80	0.81	0.81
	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 95 and name CA)	17.89	0.75	0.75
	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 95 and name CB)	18.42	0.78	0.78
45	assign (segid 3A4 and resid 82 and name CA) (segid 3A4 and resid 97 and name CB)	17.71	1.07	1.07
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 130 and name CA)	17.98	0.70	0.71
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 130 and name CB)	18.36	0.79	0.78
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 131 and name CA)	18.19	0.81	0.82
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 133 and name CA)	15.30	1.47	1.47
50	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 133 and name CB)	15.22	1.55	1.55
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 134 and name CA)	14.02	1.08	1.08
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 135 and name CA)	15.43	0.94	0.93
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 135 and name CB)	16.70	0.92	0.91
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 136 and name CA)	14.54	1.51	1.52
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 136 and name CB)	14.82	1.99	1.98
55	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 137 and name CA)	11.75	0.95	0.95
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 137 and name CB)	12.24	1.51	1.52
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 138 and name CA)	12.54	1.57	1.58
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 138 and name CB)	15.21	1.29	1.28
60	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 140 and name CA)	17.47	1.11	1.11
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 140 and name CB)	17.32	1.22	1.23
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 194 and name CB)	18.32	0.91	0.92
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 195 and name CA)	18.14	0.81	0.81
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 198 and name CA)	16.13	0.63	0.63
65	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 198 and name CB)	15.09	0.63	0.62
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 199 and name CA)	17.57	0.56	0.55
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 199 and name CB)	18.57	0.54	0.55
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 201 and name CA)	17.28	0.79	0.80
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 201 and name CB)	16.39	0.78	0.78
70	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 202 and name CA)	15.32	0.73	0.73
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 202 and name CB)	14.80	0.64	0.64
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 205 and name CA)	16.82	1.01	1.02
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 205 and name CB)	15.43	1.02	1.02
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 206 and name CA)	17.60	0.93	0.94
75	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 206 and name CB)	17.78	0.91	0.90
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 219 and name CA)	11.83	1.12	1.12
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 219 and name CB)	12.59	1.00	1.00
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 220 and name CA)	8.31	0.99	0.99
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 220 and name CB)	7.66	1.00	0.99
80	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 221 and name CA)	10.00	0.70	0.70
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 221 and name CB)	11.21	0.69	0.68
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 222 and name CA)	11.91	0.82	0.82
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 222 and name CB)	12.86	0.86	0.86

	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 223 and name CA)	9.35	0.96	0.95
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 223 and name CB)	8.43	1.08	1.09
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 224 and name CA)	7.96	0.77	0.77
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 224 and name CB)	7.47	0.82	0.83
5	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 225 and name CA)	11.61	0.81	0.81
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 225 and name CB)	12.59	0.74	0.73
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 226 and name CA)	12.75	0.83	0.83
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 240 and name CA)	14.07	0.76	0.77
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 240 and name CB)	14.85	0.72	0.72
10	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 241 and name CA)	14.65	0.51	0.51
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 241 and name CB)	16.04	0.51	0.51
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 242 and name CA)	14.69	0.50	0.50
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 242 and name CB)	15.71	0.55	0.54
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 243 and name CA)	11.34	0.53	0.54
15	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 243 and name CB)	11.03	0.60	0.60
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 244 and name CA)	9.91	0.41	0.40
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 244 and name CB)	10.62	0.43	0.42
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 245 and name CA)	12.16	0.40	0.40
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 245 and name CB)	13.63	0.38	0.39
20	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 246 and name CA)	11.34	0.52	0.52
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 246 and name CB)	11.70	0.48	0.47
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 247 and name CA)	7.67	0.53	0.54
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 247 and name CB)	6.62	0.52	0.53
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 248 and name CA)	9.21	0.73	0.72
25	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 248 and name CB)	10.15	0.73	0.73
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 249 and name CA)	11.88	0.71	0.72
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 250 and name CA)	10.17	0.74	0.73
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 250 and name CB)	9.34	0.75	0.75
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 251 and name CA)	8.66	0.74	0.73
30	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 251 and name CB)	7.77	0.77	0.78
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 252 and name CA)	12.22	0.75	0.75
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 252 and name CB)	12.95	0.77	0.78
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 253 and name CA)	14.10	0.79	0.78
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 254 and name CA)	12.59	0.75	0.74
35	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 255 and name CA)	12.91	0.70	0.70
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 256 and name CA)	16.08	0.60	0.60
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 257 and name CA)	18.45	0.94	0.94
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 258 and name CA)	17.82	0.90	0.90
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 258 and name CB)	16.63	0.98	0.98
40	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 259 and name CA)	18.09	0.57	0.57
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 259 and name CB)	17.19	0.52	0.53
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 319 and name CB)	18.78	0.57	0.57
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 384 and name CA)	16.01	0.74	0.75
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 384 and name CB)	15.41	0.75	0.75
45	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 385 and name CA)	16.69	0.79	0.80
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 386 and name CA)	17.17	0.77	0.76
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 387 and name CA)	16.17	0.75	0.74
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 388 and name CA)	13.26	0.75	0.75
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 388 and name CB)	13.57	0.75	0.75
50	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 389 and name CA)	11.99	0.80	0.81
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 389 and name CB)	12.81	0.88	0.87
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 390 and name CA)	12.58	0.81	0.80
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 390 and name CB)	13.09	0.80	0.80
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 391 and name CA)	10.93	0.76	0.76
55	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 391 and name CB)	11.93	0.75	0.74
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 392 and name CA)	7.68	0.65	0.64
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 392 and name CB)	6.32	0.65	0.64
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 393 and name CA)	9.33	0.58	0.59
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 394 and name CA)	12.56	0.66	0.66
60	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 394 and name CB)	12.95	0.71	0.70
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 395 and name CA)	13.13	0.74	0.74
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 396 and name CA)	12.78	0.68	0.68
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 396 and name CB)	11.65	0.68	0.68
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 397 and name CA)	14.88	0.64	0.64
65	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 397 and name CB)	14.70	0.64	0.65
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 398 and name CA)	17.46	0.69	0.68
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 398 and name CB)	17.48	0.70	0.70
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 399 and name CA)	17.80	0.70	0.69
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 399 and name CB)	16.87	0.72	0.71
70	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 400 and name CA)	17.54	0.70	0.70
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 83 and name C)	5.46	0.08	0.07
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 83 and name CB)	4.57	0.08	0.07
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 83 and name N)	5.53	0.14	0.13
75	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 83 and name O)	3.28	0.10	0.09
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 84 and name C)	6.27	0.19	0.19
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 84 and name CA)	6.97	0.15	0.15
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 84 and name CB)	6.83	0.12	0.11
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 84 and name N)	7.34	0.23	0.23
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 84 and name O)	5.67	0.14	0.13
80	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 85 and name C)	6.82	0.41	0.40
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 85 and name CA)	6.57	0.36	0.35
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 85 and name CB)	6.04	0.53	0.54
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 85 and name N)	6.08	0.21	0.22

	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 86 and name CA)	6.83	0.51	0.51
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 86 and name CB)	6.10	0.57	0.58
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 86 and name N)	6.19	0.45	0.45
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 94 and name CA)	15.05	0.99	0.99
5	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 94 and name CB)	13.98	0.89	0.89
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 95 and name CA)	18.12	0.75	0.75
	assign (segid 3A4 and resid 82 and name CB) (segid 3A4 and resid 95 and name CB)	18.72	0.77	0.77
	assign (segid 3A4 and resid 82 and name N) (segid 3A4 and resid 82 and name C)	2.51	0.04	0.03
	assign (segid 3A4 and resid 82 and name N) (segid 3A4 and resid 82 and name CA)	1.47	0.02	0.01
10	assign (segid 3A4 and resid 82 and name N) (segid 3A4 and resid 82 and name CB)	2.46	0.03	0.03
	assign (segid 3A4 and resid 82 and name N) (segid 3A4 and resid 82 and name O)	3.58	0.07	0.06
	assign (segid 3A4 and resid 82 and name N) (segid 3A4 and resid 83 and name C)	4.94	0.17	0.16
	assign (segid 3A4 and resid 82 and name N) (segid 3A4 and resid 83 and name CA)	4.24	0.05	0.05
	assign (segid 3A4 and resid 82 and name N) (segid 3A4 and resid 83 and name CB)	4.90	0.08	0.07
15	assign (segid 3A4 and resid 82 and name N) (segid 3A4 and resid 83 and name N)	2.82	0.05	0.06
	assign (segid 3A4 and resid 82 and name N) (segid 3A4 and resid 83 and name O)	6.03	0.12	0.13
	assign (segid 3A4 and resid 82 and name N) (segid 3A4 and resid 84 and name C)	6.33	0.46	0.46
	assign (segid 3A4 and resid 82 and name N) (segid 3A4 and resid 84 and name CA)	5.82	0.45	0.44
	assign (segid 3A4 and resid 82 and name N) (segid 3A4 and resid 84 and name CB)	5.93	0.56	0.56
20	assign (segid 3A4 and resid 82 and name N) (segid 3A4 and resid 84 and name N)	4.69	0.37	0.36
	assign (segid 3A4 and resid 82 and name N) (segid 3A4 and resid 85 and name CA)	6.54	0.49	0.48
	assign (segid 3A4 and resid 82 and name N) (segid 3A4 and resid 85 and name CB)	6.14	0.50	0.50
	assign (segid 3A4 and resid 82 and name N) (segid 3A4 and resid 85 and name N)	5.67	0.45	0.45
	assign (segid 3A4 and resid 82 and name N) (segid 3A4 and resid 86 and name N)	6.73	0.53	0.53
25	assign (segid 3A4 and resid 82 and name O) (segid 3A4 and resid 392 and name CB)	6.61	0.65	0.64
	assign (segid 3A4 and resid 82 and name O) (segid 3A4 and resid 82 and name CB)	3.20	0.11	0.10
	assign (segid 3A4 and resid 82 and name O) (segid 3A4 and resid 83 and name CA)	2.89	0.09	0.10
	assign (segid 3A4 and resid 82 and name O) (segid 3A4 and resid 83 and name CB)	2.79	0.02	0.02
	assign (segid 3A4 and resid 82 and name O) (segid 3A4 and resid 83 and name N)	4.26	0.02	0.02
30	assign (segid 3A4 and resid 82 and name O) (segid 3A4 and resid 83 and name O)	2.25	0.01	0.01
	assign (segid 3A4 and resid 82 and name O) (segid 3A4 and resid 84 and name C)	3.47	0.18	0.18
	assign (segid 3A4 and resid 82 and name O) (segid 3A4 and resid 84 and name CA)	3.99	0.19	0.19
	assign (segid 3A4 and resid 82 and name O) (segid 3A4 and resid 84 and name CB)	4.11	0.14	0.14
	assign (segid 3A4 and resid 82 and name O) (segid 3A4 and resid 84 and name N)	4.99	0.12	0.13
35	assign (segid 3A4 and resid 82 and name O) (segid 3A4 and resid 84 and name O)	3.18	0.11	0.11
	assign (segid 3A4 and resid 82 and name O) (segid 3A4 and resid 85 and name C)	5.04	0.25	0.25
	assign (segid 3A4 and resid 82 and name O) (segid 3A4 and resid 85 and name CA)	3.99	0.35	0.35
	assign (segid 3A4 and resid 82 and name O) (segid 3A4 and resid 85 and name CB)	3.80	0.31	0.32
40	assign (segid 3A4 and resid 82 and name O) (segid 3A4 and resid 85 and name N)	3.87	0.40	0.40
	assign (segid 3A4 and resid 82 and name O) (segid 3A4 and resid 85 and name O)	3.18	0.28	0.27
	assign (segid 3A4 and resid 82 and name O) (segid 3A4 and resid 86 and name C)	5.10	0.35	0.36
	assign (segid 3A4 and resid 82 and name O) (segid 3A4 and resid 86 and name CA)	5.13	0.57	0.58
	assign (segid 3A4 and resid 82 and name O) (segid 3A4 and resid 86 and name CB)	4.23	0.49	0.50
45	assign (segid 3A4 and resid 82 and name O) (segid 3A4 and resid 86 and name N)	4.03	0.49	0.50
	assign (segid 3A4 and resid 82 and name O) (segid 3A4 and resid 86 and name O)	3.31	0.43	0.44
	assign (segid 3A4 and resid 83 and name C) (segid 3A4 and resid 86 and name O)	5.93	0.77	0.77
	assign (segid 3A4 and resid 83 and name C) (segid 3A4 and resid 83 and name CB)	2.51	0.03	0.02
	assign (segid 3A4 and resid 83 and name C) (segid 3A4 and resid 84 and name C)	1.24	0.01	0.00
50	assign (segid 3A4 and resid 83 and name C) (segid 3A4 and resid 84 and name CA)	3.10	0.06	0.05
	assign (segid 3A4 and resid 83 and name C) (segid 3A4 and resid 84 and name CB)	2.42	0.03	0.03
	assign (segid 3A4 and resid 83 and name C) (segid 3A4 and resid 84 and name N)	3.66	0.06	0.06
	assign (segid 3A4 and resid 83 and name C) (segid 3A4 and resid 84 and name O)	1.33	0.01	0.01
	assign (segid 3A4 and resid 83 and name C) (segid 3A4 and resid 85 and name C)	4.00	0.11	0.11
55	assign (segid 3A4 and resid 83 and name C) (segid 3A4 and resid 85 and name CA)	4.70	0.13	0.12
	assign (segid 3A4 and resid 83 and name C) (segid 3A4 and resid 85 and name CB)	4.53	0.18	0.18
	assign (segid 3A4 and resid 83 and name C) (segid 3A4 and resid 85 and name N)	5.39	0.23	0.23
	assign (segid 3A4 and resid 83 and name C) (segid 3A4 and resid 85 and name O)	3.31	0.18	0.19
	assign (segid 3A4 and resid 83 and name C) (segid 3A4 and resid 86 and name C)	5.85	0.16	0.15
60	assign (segid 3A4 and resid 83 and name C) (segid 3A4 and resid 86 and name CA)	4.86	0.14	0.14
	assign (segid 3A4 and resid 83 and name C) (segid 3A4 and resid 86 and name CB)	4.76	0.12	0.13
	assign (segid 3A4 and resid 83 and name C) (segid 3A4 and resid 86 and name N)	4.94	0.37	0.37
	assign (segid 3A4 and resid 83 and name C) (segid 3A4 and resid 86 and name O)	3.96	0.10	0.11
	assign (segid 3A4 and resid 83 and name C) (segid 3A4 and resid 133 and name CA)	5.58	0.51	0.50
65	assign (segid 3A4 and resid 83 and name C) (segid 3A4 and resid 133 and name CB)	16.68	1.11	1.12
	assign (segid 3A4 and resid 83 and name C) (segid 3A4 and resid 134 and name CA)	16.45	1.08	1.08
	assign (segid 3A4 and resid 83 and name C) (segid 3A4 and resid 135 and name CA)	16.03	1.35	1.36
	assign (segid 3A4 and resid 83 and name C) (segid 3A4 and resid 136 and name CA)	17.61	0.83	0.82
	assign (segid 3A4 and resid 83 and name C) (segid 3A4 and resid 136 and name CB)	16.17	1.35	1.35
70	assign (segid 3A4 and resid 83 and name C) (segid 3A4 and resid 136 and name N)	16.13	1.87	1.87
	assign (segid 3A4 and resid 83 and name C) (segid 3A4 and resid 137 and name CA)	13.60	0.55	0.55
	assign (segid 3A4 and resid 83 and name C) (segid 3A4 and resid 138 and name CA)	14.94	1.38	1.37
	assign (segid 3A4 and resid 83 and name C) (segid 3A4 and resid 138 and name CB)	15.48	1.45	1.46
	assign (segid 3A4 and resid 83 and name C) (segid 3A4 and resid 139 and name CA)	17.59	0.92	0.93
75	assign (segid 3A4 and resid 83 and name C) (segid 3A4 and resid 202 and name CB)	18.80	0.59	0.60
	assign (segid 3A4 and resid 83 and name C) (segid 3A4 and resid 219 and name CA)	13.50	0.52	0.53
	assign (segid 3A4 and resid 83 and name C) (segid 3A4 and resid 219 and name CB)	14.58	0.48	0.48
	assign (segid 3A4 and resid 83 and name C) (segid 3A4 and resid 220 and name CA)	10.62	0.35	0.36
	assign (segid 3A4 and resid 83 and name C) (segid 3A4 and resid 220 and name CB)	10.12	0.43	0.42
	assign (segid 3A4 and resid 83 and name C) (segid 3A4 and resid 221 and name CA)	13.21	0.45	0.46
80	assign (segid 3A4 and resid 83 and name C) (segid 3A4 and resid 221 and name CB)	14.54	0.49	0.49
	assign (segid 3A4 and resid 83 and name C) (segid 3A4 and resid 222 and name CA)	14.41	0.30	0.30
	assign (segid 3A4 and resid 83 and name C) (segid 3A4 and resid 222 and name CB)	15.04	0.23	0.24
	assign (segid 3A4 and resid 83 and name C) (segid 3A4 and resid 223 and name CA)	11.22	0.37	0.37

	assign (segid 3A4 and resid 83 and name CA) (segid 3A4 and resid 223 and name CB)	9.99	0.36	0.36
	assign (segid 3A4 and resid 83 and name CA) (segid 3A4 and resid 224 and name CA)	10.95	0.71	0.71
	assign (segid 3A4 and resid 83 and name CA) (segid 3A4 and resid 224 and name CB)	10.90	0.84	0.84
	assign (segid 3A4 and resid 83 and name CA) (segid 3A4 and resid 225 and name CA)	14.67	0.74	0.75
	assign (segid 3A4 and resid 83 and name CA) (segid 3A4 and resid 225 and name CB)	15.69	0.63	0.63
5	assign (segid 3A4 and resid 83 and name CA) (segid 3A4 and resid 226 and name CA)	14.86	0.73	0.74
	assign (segid 3A4 and resid 83 and name CA) (segid 3A4 and resid 240 and name CA)	17.70	0.70	0.70
	assign (segid 3A4 and resid 83 and name CA) (segid 3A4 and resid 240 and name CB)	18.49	0.66	0.66
	assign (segid 3A4 and resid 83 and name CA) (segid 3A4 and resid 241 and name CA)	18.68	0.41	0.40
	assign (segid 3A4 and resid 83 and name CA) (segid 3A4 and resid 242 and name CA)	18.91	0.39	0.39
10	assign (segid 3A4 and resid 83 and name CA) (segid 3A4 and resid 243 and name CA)	15.45	0.44	0.43
	assign (segid 3A4 and resid 83 and name CA) (segid 3A4 and resid 243 and name CB)	14.92	0.50	0.49
	assign (segid 3A4 and resid 83 and name CA) (segid 3A4 and resid 244 and name CA)	14.14	0.33	0.34
	assign (segid 3A4 and resid 83 and name CA) (segid 3A4 and resid 244 and name CB)	14.73	0.38	0.38
	assign (segid 3A4 and resid 83 and name CA) (segid 3A4 and resid 245 and name CA)	16.57	0.38	0.37
15	assign (segid 3A4 and resid 83 and name CA) (segid 3A4 and resid 245 and name CB)	18.05	0.36	0.35
	assign (segid 3A4 and resid 83 and name CA) (segid 3A4 and resid 246 and name CA)	15.66	0.37	0.38
	assign (segid 3A4 and resid 83 and name CA) (segid 3A4 and resid 246 and name CB)	15.94	0.27	0.27
	assign (segid 3A4 and resid 83 and name CA) (segid 3A4 and resid 247 and name CA)	11.99	0.45	0.45
	assign (segid 3A4 and resid 83 and name CA) (segid 3A4 and resid 247 and name CB)	10.98	0.47	0.47
20	assign (segid 3A4 and resid 83 and name CA) (segid 3A4 and resid 248 and name CA)	13.36	0.74	0.74
	assign (segid 3A4 and resid 83 and name CA) (segid 3A4 and resid 248 and name CB)	14.31	0.78	0.77
	assign (segid 3A4 and resid 83 and name CA) (segid 3A4 and resid 249 and name CA)	15.92	0.69	0.69
	assign (segid 3A4 and resid 83 and name CA) (segid 3A4 and resid 250 and name CA)	13.79	0.66	0.65
	assign (segid 3A4 and resid 83 and name CA) (segid 3A4 and resid 250 and name CB)	12.98	0.65	0.64
25	assign (segid 3A4 and resid 83 and name CA) (segid 3A4 and resid 251 and name CA)	11.81	0.77	0.78
	assign (segid 3A4 and resid 83 and name CA) (segid 3A4 and resid 251 and name CB)	11.03	0.83	0.82
	assign (segid 3A4 and resid 83 and name CA) (segid 3A4 and resid 252 and name CA)	15.34	0.81	0.81
	assign (segid 3A4 and resid 83 and name CA) (segid 3A4 and resid 252 and name CB)	16.32	0.82	0.82
	assign (segid 3A4 and resid 83 and name CA) (segid 3A4 and resid 253 and name CA)	17.07	0.78	0.79
30	assign (segid 3A4 and resid 83 and name CA) (segid 3A4 and resid 254 and name CA)	14.83	0.77	0.77
	assign (segid 3A4 and resid 83 and name CA) (segid 3A4 and resid 255 and name CA)	14.63	0.64	0.64
	assign (segid 3A4 and resid 83 and name CA) (segid 3A4 and resid 256 and name CA)	18.02	0.67	0.67
	assign (segid 3A4 and resid 83 and name CA) (segid 3A4 and resid 258 and name CA)	18.92	0.79	0.78
	assign (segid 3A4 and resid 83 and name CA) (segid 3A4 and resid 258 and name CB)	17.63	0.86	0.87
35	assign (segid 3A4 and resid 83 and name CA) (segid 3A4 and resid 259 and name CA)	18.75	0.65	0.65
	assign (segid 3A4 and resid 83 and name CA) (segid 3A4 and resid 259 and name CB)	17.85	0.64	0.65
	assign (segid 3A4 and resid 83 and name CA) (segid 3A4 and resid 384 and name CA)	15.12	0.63	0.62
	assign (segid 3A4 and resid 83 and name CA) (segid 3A4 and resid 384 and name CB)	14.21	0.72	0.73
	assign (segid 3A4 and resid 83 and name CA) (segid 3A4 and resid 385 and name CA)	15.90	0.44	0.43
40	assign (segid 3A4 and resid 83 and name CA) (segid 3A4 and resid 386 and name CA)	15.72	0.73	0.74
	assign (segid 3A4 and resid 83 and name CA) (segid 3A4 and resid 387 and name CA)	14.60	0.81	0.82
	assign (segid 3A4 and resid 83 and name CA) (segid 3A4 and resid 388 and name CA)	11.96	0.79	0.80
	assign (segid 3A4 and resid 83 and name CA) (segid 3A4 and resid 388 and name CB)	12.45	0.83	0.83
	assign (segid 3A4 and resid 83 and name CA) (segid 3A4 and resid 389 and name CA)	11.69	0.40	0.40
45	assign (segid 3A4 and resid 83 and name CA) (segid 3A4 and resid 389 and name CB)	12.89	0.35	0.35
	assign (segid 3A4 and resid 83 and name CA) (segid 3A4 and resid 390 and name CA)	11.46	0.50	0.50
	assign (segid 3A4 and resid 83 and name CA) (segid 3A4 and resid 390 and name CB)	11.46	0.55	0.56
	assign (segid 3A4 and resid 83 and name CA) (segid 3A4 and resid 391 and name CA)	10.36	0.55	0.55
	assign (segid 3A4 and resid 83 and name CA) (segid 3A4 and resid 391 and name CB)	11.38	0.62	0.61
50	assign (segid 3A4 and resid 83 and name CA) (segid 3A4 and resid 392 and name CA)	6.81	0.55	0.54
	assign (segid 3A4 and resid 83 and name CA) (segid 3A4 and resid 392 and name CB)	6.09	0.54	0.54
	assign (segid 3A4 and resid 83 and name CA) (segid 3A4 and resid 392 and name O)	6.53	0.65	0.66
	assign (segid 3A4 and resid 83 and name CA) (segid 3A4 and resid 393 and name CA)	8.88	0.63	0.62
	assign (segid 3A4 and resid 83 and name CA) (segid 3A4 and resid 394 and name CA)	11.10	0.69	0.68
55	assign (segid 3A4 and resid 83 and name CA) (segid 3A4 and resid 394 and name CB)	11.16	0.72	0.72
	assign (segid 3A4 and resid 83 and name CA) (segid 3A4 and resid 395 and name CA)	10.97	0.75	0.76
	assign (segid 3A4 and resid 83 and name CA) (segid 3A4 and resid 396 and name CA)	11.72	0.67	0.68
	assign (segid 3A4 and resid 83 and name CA) (segid 3A4 and resid 396 and name CB)	11.01	0.66	0.66
	assign (segid 3A4 and resid 83 and name CA) (segid 3A4 and resid 397 and name CA)	14.26	0.74	0.73
60	assign (segid 3A4 and resid 83 and name CA) (segid 3A4 and resid 397 and name CB)	14.16	0.75	0.75
	assign (segid 3A4 and resid 83 and name CA) (segid 3A4 and resid 398 and name CA)	15.98	0.75	0.74
	assign (segid 3A4 and resid 83 and name CA) (segid 3A4 and resid 398 and name CB)	15.66	0.76	0.76
	assign (segid 3A4 and resid 83 and name CA) (segid 3A4 and resid 399 and name CA)	16.31	0.64	0.64
	assign (segid 3A4 and resid 83 and name CA) (segid 3A4 and resid 399 and name CB)	15.34	0.59	0.59
65	assign (segid 3A4 and resid 83 and name CA) (segid 3A4 and resid 400 and name CA)	17.84	0.66	0.66
	assign (segid 3A4 and resid 83 and name CA) (segid 3A4 and resid 400 and name CB)	17.28	0.65	0.65
	assign (segid 3A4 and resid 83 and name CA) (segid 3A4 and resid 83 and name C)	1.53	0.02	0.01
	assign (segid 3A4 and resid 83 and name CA) (segid 3A4 and resid 83 and name CB)	1.52	0.00	0.01
	assign (segid 3A4 and resid 83 and name CA) (segid 3A4 and resid 83 and name O)	2.40	0.02	0.01
70	assign (segid 3A4 and resid 83 and name CA) (segid 3A4 and resid 84 and name C)	4.51	0.07	0.06
	assign (segid 3A4 and resid 83 and name CA) (segid 3A4 and resid 84 and name CA)	3.82	0.04	0.03
	assign (segid 3A4 and resid 83 and name CA) (segid 3A4 and resid 84 and name CB)	4.84	0.04	0.04
	assign (segid 3A4 and resid 83 and name CA) (segid 3A4 and resid 84 and name N)	2.46	0.03	0.04
	assign (segid 3A4 and resid 83 and name CA) (segid 3A4 and resid 84 and name O)	5.48	0.13	0.13
75	assign (segid 3A4 and resid 83 and name CA) (segid 3A4 and resid 85 and name C)	5.63	0.18	0.18
	assign (segid 3A4 and resid 83 and name CA) (segid 3A4 and resid 85 and name CA)	5.57	0.19	0.18
	assign (segid 3A4 and resid 83 and name CA) (segid 3A4 and resid 85 and name CB)	6.16	0.26	0.25
	assign (segid 3A4 and resid 83 and name CA) (segid 3A4 and resid 85 and name N)	4.46	0.17	0.17
	assign (segid 3A4 and resid 83 and name CA) (segid 3A4 and resid 85 and name O)	6.78	0.20	0.20
80	assign (segid 3A4 and resid 83 and name CA) (segid 3A4 and resid 86 and name C)	5.52	0.35	0.31
	assign (segid 3A4 and resid 83 and name CA) (segid 3A4 and resid 86 and name CA)	5.31	0.13	0.13
	assign (segid 3A4 and resid 83 and name CA) (segid 3A4 and resid 86 and name CB)	5.06	0.28	0.28

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	assign (segid 3A4 and resid 83 and name CA) (segid 3A4 and resid 86 and name N)	4.71	0.12	0.12
	assign (segid 3A4 and resid 83 and name CA) (segid 3A4 and resid 86 and name O)	6.06	0.72	0.72
	assign (segid 3A4 and resid 83 and name CA) (segid 3A4 and resid 91 and name CA)	14.15	1.06	1.06
	assign (segid 3A4 and resid 83 and name CA) (segid 3A4 and resid 94 and name CB)	13.14	1.02	1.02
	assign (segid 3A4 and resid 83 and name CA) (segid 3A4 and resid 95 and name CA)	16.75	1.02	1.03
5	assign (segid 3A4 and resid 83 and name CA) (segid 3A4 and resid 95 and name CB)	17.02	1.08	1.09
	assign (segid 3A4 and resid 83 and name CA) (segid 3A4 and resid 97 and name CB)	17.76	1.18	1.19
	assign (segid 3A4 and resid 83 and name CA) (segid 3A4 and resid 98 and name CA)	18.79	0.57	0.58
	assign (segid 3A4 and resid 83 and name CA) (segid 3A4 and resid 98 and name CB)	18.02	0.60	0.60
10	assign (segid 3A4 and resid 83 and name CB) (segid 3A4 and resid 133 and name CA)	18.04	1.09	1.08
	assign (segid 3A4 and resid 83 and name CB) (segid 3A4 and resid 133 and name CB)	17.74	1.05	1.06
	assign (segid 3A4 and resid 83 and name CB) (segid 3A4 and resid 136 and name CA)	17.65	1.32	1.33
	assign (segid 3A4 and resid 83 and name CB) (segid 3A4 and resid 136 and name CB)	17.60	1.85	1.84
	assign (segid 3A4 and resid 83 and name CB) (segid 3A4 and resid 137 and name CA)	15.07	0.52	0.53
15	assign (segid 3A4 and resid 83 and name CB) (segid 3A4 and resid 138 and name CA)	16.39	1.37	1.38
	assign (segid 3A4 and resid 83 and name CB) (segid 3A4 and resid 138 and name CB)	16.91	1.45	1.46
	assign (segid 3A4 and resid 83 and name CB) (segid 3A4 and resid 219 and name CA)	14.96	0.55	0.54
	assign (segid 3A4 and resid 83 and name CB) (segid 3A4 and resid 219 and name CB)	16.05	0.49	0.49
20	assign (segid 3A4 and resid 83 and name CB) (segid 3A4 and resid 220 and name CA)	12.06	0.37	0.36
	assign (segid 3A4 and resid 83 and name CB) (segid 3A4 and resid 220 and name CB)	11.57	0.42	0.42
	assign (segid 3A4 and resid 83 and name CB) (segid 3A4 and resid 221 and name CA)	14.53	0.41	0.42
	assign (segid 3A4 and resid 83 and name CB) (segid 3A4 and resid 221 and name CB)	15.88	0.45	0.45
	assign (segid 3A4 and resid 83 and name CB) (segid 3A4 and resid 222 and name CA)	15.66	0.32	0.32
	assign (segid 3A4 and resid 83 and name CB) (segid 3A4 and resid 222 and name CB)	16.32	0.29	0.29
25	assign (segid 3A4 and resid 83 and name CB) (segid 3A4 and resid 223 and name CA)	12.36	0.10	0.41
	assign (segid 3A4 and resid 83 and name CB) (segid 3A4 and resid 223 and name CB)	11.19	0.42	0.42
	assign (segid 3A4 and resid 83 and name CB) (segid 3A4 and resid 224 and name CA)	11.96	0.62	0.63
	assign (segid 3A4 and resid 83 and name CB) (segid 3A4 and resid 224 and name CB)	11.96	0.76	0.75
30	assign (segid 3A4 and resid 83 and name CB) (segid 3A4 and resid 225 and name CA)	15.64	0.68	0.68
	assign (segid 3A4 and resid 83 and name CB) (segid 3A4 and resid 225 and name CB)	16.73	0.57	0.57
	assign (segid 3A4 and resid 83 and name CB) (segid 3A4 and resid 226 and name CA)	15.69	0.70	0.69
	assign (segid 3A4 and resid 83 and name CB) (segid 3A4 and resid 226 and name CB)	18.15	0.60	0.61
35	assign (segid 3A4 and resid 83 and name CB) (segid 3A4 and resid 240 and name CA)	18.88	0.60	0.59
	assign (segid 3A4 and resid 83 and name CB) (segid 3A4 and resid 241 and name CA)	19.39	0.33	0.32
	assign (segid 3A4 and resid 83 and name CB) (segid 3A4 and resid 243 and name CA)	15.96	0.41	0.40
	assign (segid 3A4 and resid 83 and name CB) (segid 3A4 and resid 243 and name CB)	15.33	0.46	0.45
	assign (segid 3A4 and resid 83 and name CB) (segid 3A4 and resid 244 and name CA)	14.96	0.26	0.26
40	assign (segid 3A4 and resid 83 and name CB) (segid 3A4 and resid 244 and name CB)	15.60	0.31	0.30
	assign (segid 3A4 and resid 83 and name CB) (segid 3A4 and resid 245 and name CA)	17.48	0.34	0.33
	assign (segid 3A4 and resid 83 and name CB) (segid 3A4 and resid 245 and name CB)	18.93	0.30	0.31
	assign (segid 3A4 and resid 83 and name CB) (segid 3A4 and resid 246 and name CA)	16.38	0.36	0.36
	assign (segid 3A4 and resid 83 and name CB) (segid 3A4 and resid 246 and name CB)	16.53	0.27	0.27
	assign (segid 3A4 and resid 83 and name CB) (segid 3A4 and resid 247 and name CA)	12.79	0.45	0.46
45	assign (segid 3A4 and resid 83 and name CB) (segid 3A4 and resid 247 and name CB)	11.79	0.47	0.47
	assign (segid 3A4 and resid 83 and name CB) (segid 3A4 and resid 248 and name CA)	14.48	0.74	0.73
	assign (segid 3A4 and resid 83 and name CB) (segid 3A4 and resid 248 and name CB)	15.46	0.74	0.75
	assign (segid 3A4 and resid 83 and name CB) (segid 3A4 and resid 249 and name CA)	16.91	0.69	0.69
	assign (segid 3A4 and resid 83 and name CB) (segid 3A4 and resid 250 and name CA)	14.59	0.66	0.67
	assign (segid 3A4 and resid 83 and name CB) (segid 3A4 and resid 250 and name CB)	13.67	0.64	0.65
50	assign (segid 3A4 and resid 83 and name CB) (segid 3A4 and resid 251 and name CA)	12.88	0.79	0.78
	assign (segid 3A4 and resid 83 and name CB) (segid 3A4 and resid 251 and name CB)	12.19	0.83	0.84
	assign (segid 3A4 and resid 83 and name CB) (segid 3A4 and resid 252 and name CA)	16.48	0.81	0.82
	assign (segid 3A4 and resid 83 and name CB) (segid 3A4 and resid 252 and name CB)	17.49	0.82	0.82
	assign (segid 3A4 and resid 83 and name CB) (segid 3A4 and resid 253 and name CA)	18.00	0.78	0.79
55	assign (segid 3A4 and resid 83 and name CB) (segid 3A4 and resid 254 and name CA)	15.59	0.75	0.75
	assign (segid 3A4 and resid 83 and name CB) (segid 3A4 and resid 255 and name CA)	15.60	0.64	0.65
	assign (segid 3A4 and resid 83 and name CB) (segid 3A4 and resid 255 and name CB)	18.27	0.85	0.84
	assign (segid 3A4 and resid 83 and name CB) (segid 3A4 and resid 258 and name CA)	18.75	0.66	0.65
	assign (segid 3A4 and resid 83 and name CB) (segid 3A4 and resid 259 and name CA)	18.81	0.62	0.62
60	assign (segid 3A4 and resid 83 and name CB) (segid 3A4 and resid 259 and name CB)	18.04	0.62	0.62
	assign (segid 3A4 and resid 83 and name CB) (segid 3A4 and resid 384 and name CA)	15.04	0.62	0.62
	assign (segid 3A4 and resid 83 and name CB) (segid 3A4 and resid 384 and name CB)	14.14	0.69	0.70
	assign (segid 3A4 and resid 83 and name CB) (segid 3A4 and resid 385 and name CA)	15.53	0.45	0.45
	assign (segid 3A4 and resid 83 and name CB) (segid 3A4 and resid 386 and name CA)	15.03	0.73	0.73
65	assign (segid 3A4 and resid 83 and name CB) (segid 3A4 and resid 387 and name CA)	13.66	0.79	0.78
	assign (segid 3A4 and resid 83 and name CB) (segid 3A4 and resid 388 and name CA)	10.94	0.80	0.79
	assign (segid 3A4 and resid 83 and name CB) (segid 3A4 and resid 388 and name CB)	11.36	0.86	0.86
	assign (segid 3A4 and resid 83 and name CB) (segid 3A4 and resid 389 and name CA)	11.05	0.42	0.42
	assign (segid 3A4 and resid 83 and name CB) (segid 3A4 and resid 389 and name CB)	12.31	0.36	0.37
70	assign (segid 3A4 and resid 83 and name CB) (segid 3A4 and resid 390 and name CA)	10.96	0.51	0.50
	assign (segid 3A4 and resid 83 and name CB) (segid 3A4 and resid 390 and name CB)	10.86	0.55	0.56
	assign (segid 3A4 and resid 83 and name CB) (segid 3A4 and resid 391 and name CA)	10.36	0.58	0.57
	assign (segid 3A4 and resid 83 and name CB) (segid 3A4 and resid 391 and name CB)	11.48	0.65	0.64
	assign (segid 3A4 and resid 83 and name CB) (segid 3A4 and resid 392 and name CA)	7.05	0.56	0.55
	assign (segid 3A4 and resid 83 and name CB) (segid 3A4 and resid 392 and name CB)	6.43	0.57	0.57
75	assign (segid 3A4 and resid 83 and name CB) (segid 3A4 and resid 393 and name CA)	9.58	0.62	0.63
	assign (segid 3A4 and resid 83 and name CB) (segid 3A4 and resid 394 and name CA)	11.45	0.68	0.68
	assign (segid 3A4 and resid 83 and name CB) (segid 3A4 and resid 394 and name CB)	11.31	0.71	0.72
	assign (segid 3A4 and resid 83 and name CB) (segid 3A4 and resid 395 and name CA)	11.48	0.74	0.73
	assign (segid 3A4 and resid 83 and name CB) (segid 3A4 and resid 396 and name CA)	12.63	0.64	0.63
80	assign (segid 3A4 and resid 83 and name CB) (segid 3A4 and resid 396 and name CB)	12.02	0.61	0.62
	assign (segid 3A4 and resid 83 and name CB) (segid 3A4 and resid 397 and name CA)	15.01	0.72	0.71
	assign (segid 3A4 and resid 83 and name CB) (segid 3A4 and resid 397 and name CB)	14.83	0.75	0.74
	assign (segid 3A4 and resid 83 and name CB) (segid 3A4 and resid 398 and name CA)	16.54	0.73	0.73

	assign (segid 3A4 and resid 83 and name CB) (segid 3A4 and resid 398 and name CB)	16.11	0.75	0.74
	assign (segid 3A4 and resid 83 and name CB) (segid 3A4 and resid 399 and name CA)	17.08	0.58	0.58
	assign (segid 3A4 and resid 83 and name CB) (segid 3A4 and resid 399 and name CB)	16.16	0.52	0.52
	assign (segid 3A4 and resid 83 and name CB) (segid 3A4 and resid 400 and name CB)	18.26	0.59	0.59
5	assign (segid 3A4 and resid 83 and name CB) (segid 3A4 and resid 84 and name C)	5.52	0.03	0.04
	assign (segid 3A4 and resid 83 and name CB) (segid 3A4 and resid 84 and name CA)	4.53	0.06	0.06
	assign (segid 3A4 and resid 83 and name CB) (segid 3A4 and resid 84 and name CB)	5.37	0.16	0.16
	assign (segid 3A4 and resid 83 and name CB) (segid 3A4 and resid 84 and name N)	3.23	0.05	0.05
	assign (segid 3A4 and resid 83 and name CB) (segid 3A4 and resid 84 and name O)	6.42	0.09	0.10
	assign (segid 3A4 and resid 83 and name CB) (segid 3A4 and resid 85 and name C)	7.01	0.16	0.17
10	assign (segid 3A4 and resid 83 and name CB) (segid 3A4 and resid 85 and name CA)	6.91	0.15	0.15
	assign (segid 3A4 and resid 83 and name CB) (segid 3A4 and resid 85 and name CB)	7.56	0.22	0.22
	assign (segid 3A4 and resid 83 and name CB) (segid 3A4 and resid 85 and name N)	5.70	0.13	0.13
	assign (segid 3A4 and resid 83 and name CB) (segid 3A4 and resid 86 and name C)	6.58	0.36	0.36
	assign (segid 3A4 and resid 83 and name CB) (segid 3A4 and resid 86 and name CA)	6.59	0.17	0.18
15	assign (segid 3A4 and resid 83 and name CB) (segid 3A4 and resid 86 and name CB)	6.33	0.33	0.32
	assign (segid 3A4 and resid 83 and name CB) (segid 3A4 and resid 86 and name N)	6.09	0.13	0.13
	assign (segid 3A4 and resid 83 and name CB) (segid 3A4 and resid 86 and name O)	6.99	0.74	0.74
	assign (segid 3A4 and resid 83 and name CB) (segid 3A4 and resid 94 and name CA)	15.34	1.16	1.15
	assign (segid 3A4 and resid 83 and name CB) (segid 3A4 and resid 94 and name CB)	14.33	1.16	1.15
20	assign (segid 3A4 and resid 83 and name CB) (segid 3A4 and resid 95 and name CA)	17.79	1.18	1.18
	assign (segid 3A4 and resid 83 and name CB) (segid 3A4 and resid 95 and name CB)	17.98	1.26	1.26
	assign (segid 3A4 and resid 83 and name CB) (segid 3A4 and resid 98 and name CB)	19.15	0.62	0.61
	assign (segid 3A4 and resid 83 and name N) (segid 3A4 and resid 392 and name CB)	6.26	0.57	0.58
25	assign (segid 3A4 and resid 83 and name N) (segid 3A4 and resid 83 and name C)	2.50	0.03	0.04
	assign (segid 3A4 and resid 83 and name N) (segid 3A4 and resid 83 and name CA)	1.46	0.01	0.01
	assign (segid 3A4 and resid 83 and name N) (segid 3A4 and resid 83 and name CB)	2.43	0.02	0.02
	assign (segid 3A4 and resid 83 and name N) (segid 3A4 and resid 83 and name O)	3.54	0.05	0.06
	assign (segid 3A4 and resid 83 and name N) (segid 3A4 and resid 84 and name C)	4.91	0.13	0.13
30	assign (segid 3A4 and resid 83 and name N) (segid 3A4 and resid 84 and name CA)	4.30	0.11	0.11
	assign (segid 3A4 and resid 83 and name N) (segid 3A4 and resid 84 and name CB)	5.03	0.13	0.13
	assign (segid 3A4 and resid 83 and name N) (segid 3A4 and resid 84 and name N)	2.89	0.11	0.12
	assign (segid 3A4 and resid 83 and name N) (segid 3A4 and resid 84 and name O)	6.03	0.18	0.18
	assign (segid 3A4 and resid 83 and name N) (segid 3A4 and resid 85 and name C)	5.87	0.21	0.21
35	assign (segid 3A4 and resid 83 and name N) (segid 3A4 and resid 85 and name CA)	5.61	0.19	0.18
	assign (segid 3A4 and resid 83 and name N) (segid 3A4 and resid 85 and name CB)	5.84	0.26	0.26
	assign (segid 3A4 and resid 83 and name N) (segid 3A4 and resid 85 and name N)	4.56	0.15	0.15
	assign (segid 3A4 and resid 83 and name N) (segid 3A4 and resid 85 and name O)	7.04	0.22	0.23
	assign (segid 3A4 and resid 83 and name N) (segid 3A4 and resid 86 and name C)	6.34	0.40	0.41
40	assign (segid 3A4 and resid 83 and name N) (segid 3A4 and resid 86 and name CA)	5.82	0.26	0.27
	assign (segid 3A4 and resid 83 and name N) (segid 3A4 and resid 86 and name CB)	5.45	0.32	0.33
	assign (segid 3A4 and resid 83 and name N) (segid 3A4 and resid 86 and name N)	5.07	0.24	0.24
	assign (segid 3A4 and resid 83 and name N) (segid 3A4 and resid 86 and name O)	6.96	0.75	0.75
	assign (segid 3A4 and resid 83 and name O) (segid 3A4 and resid 83 and name CB)	3.27	0.07	0.07
45	assign (segid 3A4 and resid 83 and name O) (segid 3A4 and resid 84 and name C)	3.01	0.10	0.09
	assign (segid 3A4 and resid 83 and name O) (segid 3A4 and resid 84 and name CA)	2.72	0.07	0.06
	assign (segid 3A4 and resid 83 and name O) (segid 3A4 and resid 84 and name CB)	4.18	0.08	0.08
	assign (segid 3A4 and resid 83 and name O) (segid 3A4 and resid 84 and name N)	2.23	0.02	0.03
	assign (segid 3A4 and resid 83 and name O) (segid 3A4 and resid 84 and name O)	3.60	0.10	0.11
50	assign (segid 3A4 and resid 83 and name O) (segid 3A4 and resid 85 and name C)	4.25	0.27	0.26
	assign (segid 3A4 and resid 83 and name O) (segid 3A4 and resid 85 and name CA)	4.39	0.29	0.28
	assign (segid 3A4 and resid 83 and name O) (segid 3A4 and resid 85 and name CB)	5.47	0.35	0.36
	assign (segid 3A4 and resid 83 and name O) (segid 3A4 and resid 85 and name N)	3.38	0.27	0.28
	assign (segid 3A4 and resid 83 and name O) (segid 3A4 and resid 85 and name O)	5.29	0.26	0.25
55	assign (segid 3A4 and resid 83 and name O) (segid 3A4 and resid 86 and name C)	3.90	0.15	0.15
	assign (segid 3A4 and resid 83 and name O) (segid 3A4 and resid 86 and name CA)	4.05	0.35	0.35
	assign (segid 3A4 and resid 83 and name O) (segid 3A4 and resid 86 and name CB)	4.40	0.61	0.61
	assign (segid 3A4 and resid 83 and name O) (segid 3A4 and resid 86 and name N)	3.44	0.34	0.35
	assign (segid 3A4 and resid 83 and name O) (segid 3A4 and resid 86 and name O)	4.60	0.37	0.37
60	assign (segid 3A4 and resid 83 and name O) (segid 3A4 and resid 84 and name CB)	2.50	0.01	0.01
	assign (segid 3A4 and resid 84 and name C) (segid 3A4 and resid 84 and name O)	1.23	0.00	0.01
	assign (segid 3A4 and resid 84 and name C) (segid 3A4 and resid 85 and name C)	3.20	0.14	0.14
	assign (segid 3A4 and resid 84 and name C) (segid 3A4 and resid 85 and name CA)	2.44	0.02	0.03
	assign (segid 3A4 and resid 84 and name C) (segid 3A4 and resid 85 and name CB)	3.68	0.07	0.08
65	assign (segid 3A4 and resid 84 and name C) (segid 3A4 and resid 85 and name N)	1.33	0.02	0.01
	assign (segid 3A4 and resid 84 and name C) (segid 3A4 and resid 85 and name O)	4.19	0.15	0.14
	assign (segid 3A4 and resid 84 and name C) (segid 3A4 and resid 86 and name C)	4.85	0.27	0.28
	assign (segid 3A4 and resid 84 and name C) (segid 3A4 and resid 86 and name CA)	4.65	0.30	0.29
	assign (segid 3A4 and resid 84 and name C) (segid 3A4 and resid 86 and name CB)	5.58	0.36	0.35
	assign (segid 3A4 and resid 84 and name C) (segid 3A4 and resid 86 and name N)	3.38	0.26	0.27
70	assign (segid 3A4 and resid 84 and name C) (segid 3A4 and resid 86 and name O)	5.91	0.28	0.28
	assign (segid 3A4 and resid 84 and name CA) (segid 3A4 and resid 133 and name CA)	17.20	1.19	1.18
	assign (segid 3A4 and resid 84 and name CA) (segid 3A4 and resid 133 and name CB)	17.15	1.15	1.15
	assign (segid 3A4 and resid 84 and name CA) (segid 3A4 and resid 134 and name CA)	16.74	1.44	1.44
75	assign (segid 3A4 and resid 84 and name CA) (segid 3A4 and resid 135 and name CA)	17.83	0.96	0.95
	assign (segid 3A4 and resid 84 and name CA) (segid 3A4 and resid 136 and name CA)	15.86	1.44	1.44
	assign (segid 3A4 and resid 84 and name CA) (segid 3A4 and resid 136 and name CB)	15.81	1.86	1.86
	assign (segid 3A4 and resid 84 and name CA) (segid 3A4 and resid 137 and name CA)	13.46	0.92	0.93
	assign (segid 3A4 and resid 84 and name CA) (segid 3A4 and resid 138 and name CA)	14.93	1.40	1.40
	assign (segid 3A4 and resid 84 and name CA) (segid 3A4 and resid 138 and name CB)	15.79	1.43	1.43
80	assign (segid 3A4 and resid 84 and name CA) (segid 3A4 and resid 139 and name CA)	17.03	1.02	1.02
	assign (segid 3A4 and resid 84 and name CA) (segid 3A4 and resid 219 and name CA)	12.21	0.71	0.71
	assign (segid 3A4 and resid 84 and name CA) (segid 3A4 and resid 219 and name CB)	13.51	0.67	0.67

	assign (segid 3A4 and resid 84 and name CA) (segid 3A4 and resid 220 and name CA)	10.08	0.67	0.67
	assign (segid 3A4 and resid 84 and name CA) (segid 3A4 and resid 220 and name CB)	10.05	0.70	0.70
	assign (segid 3A4 and resid 84 and name CA) (segid 3A4 and resid 221 and name CA)	12.91	0.81	0.81
	assign (segid 3A4 and resid 84 and name CA) (segid 3A4 and resid 221 and name CB)	14.33	0.79	0.79
5	assign (segid 3A4 and resid 84 and name CA) (segid 3A4 and resid 222 and name CA)	13.18	0.63	0.63
	assign (segid 3A4 and resid 84 and name CA) (segid 3A4 and resid 222 and name CB)	13.54	0.55	0.54
	assign (segid 3A4 and resid 84 and name CA) (segid 3A4 and resid 223 and name CA)	9.74	0.66	0.67
	assign (segid 3A4 and resid 84 and name CA) (segid 3A4 and resid 223 and name CB)	8.46	0.63	0.63
	assign (segid 3A4 and resid 84 and name CA) (segid 3A4 and resid 224 and name CA)	10.57	1.18	1.18
10	assign (segid 3A4 and resid 84 and name CA) (segid 3A4 and resid 224 and name CB)	10.97	1.23	1.24
	assign (segid 3A4 and resid 84 and name CA) (segid 3A4 and resid 225 and name CA)	14.01	1.17	1.17
	assign (segid 3A4 and resid 84 and name CA) (segid 3A4 and resid 225 and name CB)	14.94	1.05	1.04
	assign (segid 3A4 and resid 84 and name CA) (segid 3A4 and resid 226 and name CA)	13.42	1.13	1.13
	assign (segid 3A4 and resid 84 and name CA) (segid 3A4 and resid 243 and name CA)	17.09	1.00	1.00
15	assign (segid 3A4 and resid 84 and name CA) (segid 3A4 and resid 243 and name CB)	16.50	1.05	1.06
	assign (segid 3A4 and resid 84 and name CA) (segid 3A4 and resid 244 and name CA)	15.26	0.98	0.99
	assign (segid 3A4 and resid 84 and name CA) (segid 3A4 and resid 244 and name CB)	15.51	1.06	1.06
	assign (segid 3A4 and resid 84 and name CA) (segid 3A4 and resid 245 and name CA)	17.96	0.90	0.91
	assign (segid 3A4 and resid 84 and name CA) (segid 3A4 and resid 246 and name CA)	17.77	0.85	0.86
20	assign (segid 3A4 and resid 84 and name CA) (segid 3A4 and resid 246 and name CB)	18.17	0.75	0.75
	assign (segid 3A4 and resid 84 and name CA) (segid 3A4 and resid 247 and name CA)	14.12	0.84	0.84
	assign (segid 3A4 and resid 84 and name CA) (segid 3A4 and resid 247 and name CB)	12.95	0.92	0.91
	assign (segid 3A4 and resid 84 and name CA) (segid 3A4 and resid 248 and name CA)	14.93	1.06	1.05
	assign (segid 3A4 and resid 84 and name CA) (segid 3A4 and resid 248 and name CB)	15.58	1.15	1.15
25	assign (segid 3A4 and resid 84 and name CA) (segid 3A4 and resid 249 and name CA)	17.97	0.93	0.94
	assign (segid 3A4 and resid 84 and name CA) (segid 3A4 and resid 250 and name CA)	16.41	0.82	0.83
	assign (segid 3A4 and resid 84 and name CA) (segid 3A4 and resid 250 and name CB)	15.77	0.81	0.80
	assign (segid 3A4 and resid 84 and name CA) (segid 3A4 and resid 251 and name CA)	14.04	0.90	0.90
	assign (segid 3A4 and resid 84 and name CA) (segid 3A4 and resid 251 and name CB)	12.98	0.96	0.95
30	assign (segid 3A4 and resid 84 and name CA) (segid 3A4 and resid 252 and name CA)	17.23	0.93	0.94
	assign (segid 3A4 and resid 84 and name CA) (segid 3A4 and resid 254 and name CA)	17.60	0.92	0.93
	assign (segid 3A4 and resid 84 and name CA) (segid 3A4 and resid 255 and name CA)	16.85	0.74	0.74
	assign (segid 3A4 and resid 84 and name CA) (segid 3A4 and resid 384 and name CB)	17.04	0.94	0.95
	assign (segid 3A4 and resid 84 and name CA) (segid 3A4 and resid 387 and name CA)	17.74	1.03	1.02
35	assign (segid 3A4 and resid 84 and name CA) (segid 3A4 and resid 388 and name CA)	15.19	0.86	0.86
	assign (segid 3A4 and resid 84 and name CA) (segid 3A4 and resid 388 and name CB)	15.62	0.86	0.86
	assign (segid 3A4 and resid 84 and name CA) (segid 3A4 and resid 389 and name CA)	15.26	0.44	0.45
	assign (segid 3A4 and resid 84 and name CA) (segid 3A4 and resid 389 and name CB)	16.50	0.39	0.38
	assign (segid 3A4 and resid 84 and name CA) (segid 3A4 and resid 390 and name CA)	14.82	0.61	0.61
40	assign (segid 3A4 and resid 84 and name CA) (segid 3A4 and resid 390 and name CB)	14.64	0.70	0.70
	assign (segid 3A4 and resid 84 and name CA) (segid 3A4 and resid 391 and name CA)	13.63	0.62	0.62
	assign (segid 3A4 and resid 84 and name CA) (segid 3A4 and resid 391 and name CB)	14.48	0.69	0.69
	assign (segid 3A4 and resid 84 and name CA) (segid 3A4 and resid 392 and name CA)	10.04	0.60	0.60
	assign (segid 3A4 and resid 84 and name CA) (segid 3A4 and resid 392 and name CB)	9.49	0.53	0.53
45	assign (segid 3A4 and resid 84 and name CA) (segid 3A4 and resid 393 and name CA)	11.26	0.78	0.78
	assign (segid 3A4 and resid 84 and name CA) (segid 3A4 and resid 394 and name CA)	13.30	0.93	0.92
	assign (segid 3A4 and resid 84 and name CA) (segid 3A4 and resid 394 and name CB)	13.47	0.97	0.96
	assign (segid 3A4 and resid 84 and name CA) (segid 3A4 and resid 395 and name CA)	12.15	1.13	1.12
	assign (segid 3A4 and resid 84 and name CA) (segid 3A4 and resid 396 and name CA)	12.70	1.13	1.13
50	assign (segid 3A4 and resid 84 and name CA) (segid 3A4 and resid 396 and name CB)	12.05	1.08	1.08
	assign (segid 3A4 and resid 84 and name CA) (segid 3A4 and resid 397 and name CA)	15.85	1.04	1.04
	assign (segid 3A4 and resid 84 and name CA) (segid 3A4 and resid 397 and name CB)	16.07	0.98	0.97
	assign (segid 3A4 and resid 84 and name CA) (segid 3A4 and resid 398 and name CB)	16.90	1.18	1.19
	assign (segid 3A4 and resid 84 and name CA) (segid 3A4 and resid 399 and name CA)	16.81	1.24	1.24
55	assign (segid 3A4 and resid 84 and name CA) (segid 3A4 and resid 399 and name CB)	15.62	1.26	1.25
	assign (segid 3A4 and resid 84 and name CA) (segid 3A4 and resid 84 and name C)	1.52	0.01	0.01
	assign (segid 3A4 and resid 84 and name CA) (segid 3A4 and resid 84 and name CB)	1.52	0.00	0.01
	assign (segid 3A4 and resid 84 and name CA) (segid 3A4 and resid 84 and name O)	2.38	0.02	0.02
	assign (segid 3A4 and resid 84 and name CA) (segid 3A4 and resid 85 and name C)	4.53	0.12	0.12
60	assign (segid 3A4 and resid 84 and name CA) (segid 3A4 and resid 85 and name CA)	3.81	0.01	0.01
	assign (segid 3A4 and resid 84 and name CA) (segid 3A4 and resid 85 and name CB)	4.83	0.07	0.07
	assign (segid 3A4 and resid 84 and name CA) (segid 3A4 and resid 85 and name N)	2.43	0.01	0.02
	assign (segid 3A4 and resid 84 and name CA) (segid 3A4 and resid 85 and name O)	5.61	0.15	0.14
	assign (segid 3A4 and resid 84 and name CA) (segid 3A4 and resid 86 and name C)	5.64	0.28	0.29
65	assign (segid 3A4 and resid 84 and name CA) (segid 3A4 and resid 86 and name CA)	5.58	0.30	0.30
	assign (segid 3A4 and resid 84 and name CA) (segid 3A4 and resid 86 and name CB)	6.26	0.41	0.42
	assign (segid 3A4 and resid 84 and name CA) (segid 3A4 and resid 86 and name N)	4.42	0.25	0.24
	assign (segid 3A4 and resid 84 and name CA) (segid 3A4 and resid 86 and name O)	6.59	0.35	0.35
	assign (segid 3A4 and resid 84 and name CA) (segid 3A4 and resid 94 and name CA)	13.08	0.50	0.50
70	assign (segid 3A4 and resid 84 and name CA) (segid 3A4 and resid 94 and name CB)	12.36	0.60	0.60
	assign (segid 3A4 and resid 84 and name CA) (segid 3A4 and resid 95 and name CA)	15.75	0.45	0.44
	assign (segid 3A4 and resid 84 and name CA) (segid 3A4 and resid 95 and name CB)	15.90	0.47	0.48
	assign (segid 3A4 and resid 84 and name CA) (segid 3A4 and resid 96 and name CA)	18.13	1.12	1.11
	assign (segid 3A4 and resid 84 and name CA) (segid 3A4 and resid 97 and name CA)	17.91	0.77	0.76
75	assign (segid 3A4 and resid 84 and name CA) (segid 3A4 and resid 97 and name CB)	16.90	0.80	0.80
	assign (segid 3A4 and resid 84 and name CA) (segid 3A4 and resid 98 and name CA)	18.42	0.58	0.58
	assign (segid 3A4 and resid 84 and name CA) (segid 3A4 and resid 98 and name CB)	17.72	0.78	0.77
	assign (segid 3A4 and resid 84 and name CB) (segid 3A4 and resid 136 and name CA)	16.55	1.42	1.41
	assign (segid 3A4 and resid 84 and name CB) (segid 3A4 and resid 136 and name CB)	16.57	1.78	1.78
80	assign (segid 3A4 and resid 84 and name CB) (segid 3A4 and resid 137 and name CA)	14.13	1.08	1.08
	assign (segid 3A4 and resid 84 and name CB) (segid 3A4 and resid 138 and name CA)	15.38	1.57	1.56
	assign (segid 3A4 and resid 84 and name CB) (segid 3A4 and resid 138 and name CB)	16.27	1.59	1.59
	assign (segid 3A4 and resid 84 and name CB) (segid 3A4 and resid 139 and name CA)	17.36	1.24	1.24

	assign (segid 3A4 and resid 84 and name CB) (segid 3A4 and resid 219 and name CA)	12.36	0.94	0.94
	assign (segid 3A4 and resid 84 and name CB) (segid 3A4 and resid 219 and name CB)	13.68	0.90	0.90
	assign (segid 3A4 and resid 84 and name CB) (segid 3A4 and resid 220 and name CA)	10.31	0.95	0.95
	assign (segid 3A4 and resid 84 and name CB) (segid 3A4 and resid 220 and name CB)	10.47	0.96	0.96
	assign (segid 3A4 and resid 84 and name CB) (segid 3A4 and resid 221 and name CA)	12.88	1.08	1.09
5	assign (segid 3A4 and resid 84 and name CB) (segid 3A4 and resid 221 and name CB)	14.35	1.07	1.06
	assign (segid 3A4 and resid 84 and name CB) (segid 3A4 and resid 222 and name CA)	12.82	0.91	0.90
	assign (segid 3A4 and resid 84 and name CB) (segid 3A4 and resid 222 and name CB)	13.18	0.82	0.82
	assign (segid 3A4 and resid 84 and name CB) (segid 3A4 and resid 223 and name CA)	9.25	0.92	0.92
	assign (segid 3A4 and resid 84 and name CB) (segid 3A4 and resid 223 and name CB)	8.10	0.92	0.91
10	assign (segid 3A4 and resid 84 and name CB) (segid 3A4 and resid 224 and name CA)	10.14	1.40	1.39
	assign (segid 3A4 and resid 84 and name CB) (segid 3A4 and resid 224 and name CB)	10.71	1.44	1.44
	assign (segid 3A4 and resid 84 and name CB) (segid 3A4 and resid 225 and name CA)	13.40	1.40	1.41
	assign (segid 3A4 and resid 84 and name CB) (segid 3A4 and resid 225 and name CB)	14.37	1.28	1.28
	assign (segid 3A4 and resid 84 and name CB) (segid 3A4 and resid 226 and name CA)	12.51	1.34	1.33
15	assign (segid 3A4 and resid 84 and name CB) (segid 3A4 and resid 243 and name CA)	16.92	1.32	1.32
	assign (segid 3A4 and resid 84 and name CB) (segid 3A4 and resid 243 and name CB)	16.25	1.35	1.36
	assign (segid 3A4 and resid 84 and name CB) (segid 3A4 and resid 244 and name CA)	15.10	1.31	1.32
	assign (segid 3A4 and resid 84 and name CB) (segid 3A4 and resid 244 and name CB)	15.26	1.40	1.39
	assign (segid 3A4 and resid 84 and name CB) (segid 3A4 and resid 246 and name CA)	17.99	1.16	1.17
20	assign (segid 3A4 and resid 84 and name CB) (segid 3A4 and resid 247 and name CA)	14.45	1.13	1.13
	assign (segid 3A4 and resid 84 and name CB) (segid 3A4 and resid 247 and name CB)	13.19	1.20	1.20
	assign (segid 3A4 and resid 84 and name CB) (segid 3A4 and resid 248 and name CA)	15.32	1.35	1.36
	assign (segid 3A4 and resid 84 and name CB) (segid 3A4 and resid 248 and name CB)	15.88	1.47	1.47
	assign (segid 3A4 and resid 84 and name CB) (segid 3A4 and resid 250 and name CA)	17.12	1.02	1.01
25	assign (segid 3A4 and resid 84 and name CB) (segid 3A4 and resid 250 and name CB)	16.43	0.96	0.97
	assign (segid 3A4 and resid 84 and name CB) (segid 3A4 and resid 251 and name CA)	14.89	1.08	1.08
	assign (segid 3A4 and resid 84 and name CB) (segid 3A4 and resid 251 and name CB)	13.77	1.17	1.16
	assign (segid 3A4 and resid 84 and name CB) (segid 3A4 and resid 254 and name CA)	18.67	0.99	1.00
	assign (segid 3A4 and resid 84 and name CB) (segid 3A4 and resid 255 and name CA)	18.01	0.82	0.83
30	assign (segid 3A4 and resid 84 and name CB) (segid 3A4 and resid 388 and name CA)	15.91	0.85	0.86
	assign (segid 3A4 and resid 84 and name CB) (segid 3A4 and resid 388 and name CB)	16.22	0.86	0.87
	assign (segid 3A4 and resid 84 and name CB) (segid 3A4 and resid 389 and name CA)	16.13	0.45	0.46
	assign (segid 3A4 and resid 84 and name CB) (segid 3A4 and resid 389 and name CB)	17.34	0.41	0.41
	assign (segid 3A4 and resid 84 and name CB) (segid 3A4 and resid 390 and name CA)	15.94	0.62	0.61
35	assign (segid 3A4 and resid 84 and name CB) (segid 3A4 and resid 390 and name CB)	15.77	0.72	0.71
	assign (segid 3A4 and resid 84 and name CB) (segid 3A4 and resid 391 and name CA)	14.89	0.57	0.58
	assign (segid 3A4 and resid 84 and name CB) (segid 3A4 and resid 391 and name CB)	15.79	0.64	0.65
	assign (segid 3A4 and resid 84 and name CB) (segid 3A4 and resid 392 and name CA)	11.33	0.57	0.56
	assign (segid 3A4 and resid 84 and name CB) (segid 3A4 and resid 392 and name CB)	10.70	0.52	0.51
40	assign (segid 3A4 and resid 84 and name CB) (segid 3A4 and resid 393 and name CA)	12.66	0.74	0.74
	assign (segid 3A4 and resid 84 and name CB) (segid 3A4 and resid 394 and name CA)	14.75	0.90	0.90
	assign (segid 3A4 and resid 84 and name CB) (segid 3A4 and resid 394 and name CB)	14.90	0.95	0.96
	assign (segid 3A4 and resid 84 and name CB) (segid 3A4 and resid 395 and name CA)	13.61	1.14	1.14
	assign (segid 3A4 and resid 84 and name CB) (segid 3A4 and resid 396 and name CA)	14.11	1.12	1.12
45	assign (segid 3A4 and resid 84 and name CB) (segid 3A4 and resid 396 and name CB)	13.43	1.08	1.07
	assign (segid 3A4 and resid 84 and name CB) (segid 3A4 and resid 397 and name CA)	17.28	1.02	1.01
	assign (segid 3A4 and resid 84 and name CB) (segid 3A4 and resid 85 and name C)	5.58	0.10	0.09
	assign (segid 3A4 and resid 84 and name CB) (segid 3A4 and resid 85 and name CA)	4.53	0.10	0.10
	assign (segid 3A4 and resid 84 and name CB) (segid 3A4 and resid 85 and name CB)	5.30	0.20	0.19
50	assign (segid 3A4 and resid 84 and name CB) (segid 3A4 and resid 85 and name N)	3.22	0.09	0.10
	assign (segid 3A4 and resid 84 and name CB) (segid 3A4 and resid 85 and name O)	6.60	0.11	0.11
	assign (segid 3A4 and resid 84 and name CB) (segid 3A4 and resid 86 and name C)	7.07	0.27	0.27
	assign (segid 3A4 and resid 84 and name CB) (segid 3A4 and resid 86 and name CA)	6.92	0.23	0.23
	assign (segid 3A4 and resid 84 and name CB) (segid 3A4 and resid 86 and name CB)	7.59	0.31	0.31
55	assign (segid 3A4 and resid 84 and name CB) (segid 3A4 and resid 86 and name N)	5.66	0.18	0.17
	assign (segid 3A4 and resid 84 and name CB) (segid 3A4 and resid 94 and name CA)	14.02	0.48	0.49
	assign (segid 3A4 and resid 84 and name CB) (segid 3A4 and resid 94 and name CB)	13.38	0.61	0.61
	assign (segid 3A4 and resid 84 and name CB) (segid 3A4 and resid 95 and name CA)	16.78	0.38	0.37
	assign (segid 3A4 and resid 84 and name CB) (segid 3A4 and resid 95 and name CB)	16.93	0.39	0.38
60	assign (segid 3A4 and resid 84 and name CB) (segid 3A4 and resid 97 and name CB)	17.76	0.78	0.78
	assign (segid 3A4 and resid 84 and name N) (segid 3A4 and resid 84 and name C)	2.50	0.04	0.03
	assign (segid 3A4 and resid 84 and name N) (segid 3A4 and resid 84 and name CA)	1.45	0.01	0.01
	assign (segid 3A4 and resid 84 and name N) (segid 3A4 and resid 84 and name CB)	2.41	0.05	0.06
	assign (segid 3A4 and resid 84 and name N) (segid 3A4 and resid 84 and name O)	3.55	0.06	0.06
65	assign (segid 3A4 and resid 84 and name N) (segid 3A4 and resid 85 and name C)	4.82	0.06	0.07
	assign (segid 3A4 and resid 84 and name N) (segid 3A4 and resid 85 and name CA)	4.25	0.07	0.08
	assign (segid 3A4 and resid 84 and name N) (segid 3A4 and resid 85 and name CB)	5.05	0.12	0.11
	assign (segid 3A4 and resid 84 and name N) (segid 3A4 and resid 85 and name N)	2.84	0.08	0.08
	assign (segid 3A4 and resid 84 and name N) (segid 3A4 and resid 85 and name O)	6.00	0.11	0.11
70	assign (segid 3A4 and resid 84 and name N) (segid 3A4 and resid 86 and name C)	5.65	0.12	0.12
	assign (segid 3A4 and resid 84 and name N) (segid 3A4 and resid 86 and name CA)	5.46	0.15	0.15
	assign (segid 3A4 and resid 84 and name N) (segid 3A4 and resid 86 and name CB)	5.82	0.33	0.33
	assign (segid 3A4 and resid 84 and name N) (segid 3A4 and resid 86 and name N)	4.39	0.11	0.12
	assign (segid 3A4 and resid 84 and name N) (segid 3A4 and resid 86 and name O)	6.50	0.44	0.44
75	assign (segid 3A4 and resid 84 and name N) (segid 3A4 and resid 84 and name CB)	3.21	0.09	0.09
	assign (segid 3A4 and resid 84 and name O) (segid 3A4 and resid 85 and name C)	3.31	0.24	0.25
	assign (segid 3A4 and resid 84 and name O) (segid 3A4 and resid 85 and name CA)	2.80	0.06	0.07
	assign (segid 3A4 and resid 84 and name O) (segid 3A4 and resid 85 and name CB)	4.21	0.11	0.12
	assign (segid 3A4 and resid 84 and name O) (segid 3A4 and resid 85 and name N)	2.25	0.02	0.02
80	assign (segid 3A4 and resid 84 and name O) (segid 3A4 and resid 85 and name O)	1.03	0.25	0.26
	assign (segid 3A4 and resid 84 and name O) (segid 3A4 and resid 86 and name C)	4.75	0.50	0.50
	assign (segid 3A4 and resid 84 and name O) (segid 3A4 and resid 86 and name CA)	4.79	0.47	0.46

	assign (segid 3A4 and resid 84 and name O) (segid 3A4 and resid 86 and name CB)	5.94	0.49	0.49
	assign (segid 3A4 and resid 84 and name O) (segid 3A4 and resid 86 and name N)	3.69	0.41	0.41
	assign (segid 3A4 and resid 84 and name O) (segid 3A4 and resid 86 and name O)	5.79	0.43	0.43
	assign (segid 3A4 and resid 85 and name C) (segid 3A4 and resid 220 and name CB)	6.90	0.79	0.79
5	assign (segid 3A4 and resid 85 and name C) (segid 3A4 and resid 85 and name CB)	2.53	0.03	0.04
	assign (segid 3A4 and resid 85 and name C) (segid 3A4 and resid 85 and name O)	1.24	0.01	0.01
	assign (segid 3A4 and resid 85 and name C) (segid 3A4 and resid 86 and name C)	3.32	0.11	0.12
	assign (segid 3A4 and resid 85 and name C) (segid 3A4 and resid 86 and name CA)	2.43	0.01	0.02
	assign (segid 3A4 and resid 85 and name C) (segid 3A4 and resid 86 and name CB)	3.58	0.06	0.07
10	assign (segid 3A4 and resid 85 and name C) (segid 3A4 and resid 86 and name N)	1.33	0.00	0.00
	assign (segid 3A4 and resid 85 and name C) (segid 3A4 and resid 86 and name O)	4.43	0.15	0.15
	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 101 and name CB)	18.39	0.77	0.77
	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 130 and name CA)	17.64	1.25	1.26
	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 131 and name CA)	17.81	1.14	1.14
15	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 132 and name CA)	16.67	1.31	1.31
	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 133 and name CA)	13.88	1.13	1.13
	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 133 and name CB)	13.98	1.13	1.13
	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 134 and name CA)	13.37	1.48	1.48
	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 135 and name CA)	14.30	0.91	0.91
20	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 135 and name CB)	15.51	1.02	1.02
	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 136 and name CA)	12.26	1.34	1.33
	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 136 and name CB)	12.26	1.70	1.69
	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 137 and name CA)	9.88	0.90	0.91
	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 138 and name CA)	11.48	1.31	1.31
25	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 138 and name CB)	12.42	1.37	1.38
	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 139 and name CA)	13.53	0.85	0.84
	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 140 and name CA)	16.60	0.97	0.98
	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 140 and name CB)	16.84	1.14	1.14
	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 198 and name CA)	18.62	0.90	0.90
30	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 198 and name CB)	17.97	0.94	0.94
	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 201 and name CA)	18.30	0.72	0.72
	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 201 and name CB)	17.42	0.66	0.66
	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 202 and name CA)	16.84	0.83	0.84
	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 202 and name CB)	16.87	0.89	0.90
35	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 205 and name CA)	16.53	0.96	0.96
	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 205 and name CB)	15.28	0.94	0.94
	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 206 and name CA)	17.77	1.02	1.02
	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 206 and name CB)	18.44	1.01	1.01
	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 219 and name CA)	8.86	0.51	0.52
40	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 219 and name CB)	10.11	0.49	0.50
	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 220 and name CA)	6.92	0.62	0.62
	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 220 and name CB)	6.85	0.70	0.71
	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 221 and name CA)	10.15	0.84	0.84
	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 221 and name CB)	11.45	0.80	0.80
45	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 222 and name CA)	10.70	0.71	0.71
	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 222 and name CB)	10.94	0.59	0.60
	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 223 and name CA)	7.82	0.89	0.89
	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 223 and name CB)	6.38	0.83	0.84
	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 224 and name CA)	9.12	1.36	1.35
50	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 224 and name CB)	9.33	1.40	1.39
	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 225 and name CA)	12.52	1.26	1.26
	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 225 and name CB)	13.15	1.14	1.15
	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 226 and name CA)	12.50	1.21	1.21
	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 243 and name CA)	16.47	0.96	0.97
55	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 243 and name CB)	16.19	1.05	1.04
	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 244 and name CA)	14.03	0.98	0.97
	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 244 and name CB)	14.17	1.03	1.02
	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 245 and name CA)	16.26	0.87	0.87
	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 245 and name CB)	17.75	0.88	0.88
60	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 246 and name CA)	16.49	0.82	0.83
	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 246 and name CB)	17.17	0.73	0.74
	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 247 and name CA)	12.84	0.80	0.80
	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 247 and name CB)	11.80	0.88	0.88
	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 248 and name CA)	12.76	0.98	0.97
65	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 248 and name CB)	13.27	1.06	1.06
	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 249 and name CA)	15.93	0.92	0.91
	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 250 and name CA)	14.83	0.92	0.93
	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 250 and name CB)	14.49	0.89	0.90
	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 251 and name CA)	11.96	1.01	1.00
70	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 251 and name CB)	10.73	1.01	1.01
	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 252 and name CA)	14.68	1.03	1.03
	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 252 and name CB)	15.47	1.01	1.02
	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 253 and name CA)	17.41	1.07	1.06
	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 254 and name CA)	15.92	1.22	1.22
75	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 255 and name CA)	14.68	1.00	1.00
	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 256 and name CA)	17.54	0.85	0.85
	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 259 and name CB)	17.56	0.93	0.94
	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 384 and name CB)	17.16	0.93	0.93
	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 388 and name CA)	17.19	0.72	0.72
	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 388 and name CB)	17.75	0.73	0.73
80	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 389 and name CA)	16.49	0.39	0.40
	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 389 and name CB)	17.59	0.44	0.44
	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 390 and name CA)	15.83	0.54	0.53

	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 390 and name CB)	15.86	0.55	0.56
	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 391 and name CA)	13.78	0.69	0.69
	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 391 and name CB)	14.36	0.73	0.74
	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 392 and name CA)	10.12	0.63	0.63
5	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 392 and name CB)	9.51	0.61	0.60
	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 393 and name CA)	10.19	0.88	0.87
	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 394 and name CA)	12.79	0.91	0.91
	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 394 and name CB)	13.37	0.85	0.85
	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 395 and name CA)	11.45	1.02	1.03
	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 396 and name CA)	10.88	1.23	1.23
10	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 396 and name CB)	9.97	1.20	1.19
	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 397 and name CA)	14.20	1.11	1.12
	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 397 and name CB)	14.63	1.03	1.03
	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 398 and name CA)	16.03	1.19	1.18
	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 398 and name CB)	16.01	1.14	1.13
15	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 399 and name CA)	15.13	1.34	1.34
	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 399 and name CB)	13.85	1.37	1.37
	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 400 and name CA)	16.33	1.33	1.33
	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 400 and name CB)	15.83	1.31	1.32
20	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 85 and name C)	1.52	0.00	0.01
	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 85 and name CB)	1.55	0.02	0.01
	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 86 and name C)	4.63	0.10	0.11
	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 86 and name CA)	3.82	0.01	0.01
	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 86 and name CB)	4.79	0.05	0.05
25	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 86 and name N)	2.45	0.01	0.01
	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 86 and name O)	5.76	0.22	0.21
	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 94 and name CA)	10.35	0.59	0.59
	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 94 and name CB)	9.62	0.66	0.67
	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 95 and name CA)	13.41	0.52	0.52
30	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 95 and name CB)	13.84	0.53	0.53
	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 96 and name CA)	15.44	1.12	1.13
	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 96 and name CB)	15.42	1.50	1.50
	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 97 and name CA)	14.79	0.76	0.77
	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 97 and name CB)	13.70	0.79	0.78
35	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 98 and name CA)	15.53	0.77	0.78
	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 98 and name CB)	15.01	1.01	1.02
	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 99 and name CA)	18.64	0.62	0.63
	assign (segid 3A4 and resid 85 and name CA) (segid 3A4 and resid 99 and name CB)	18.84	0.55	0.55
40	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 101 and name CB)	18.35	0.96	0.96
	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 130 and name CA)	17.32	1.32	1.31
	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 131 and name CA)	17.27	1.22	1.21
	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 132 and name CA)	16.21	1.30	1.31
	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 133 and name CA)	13.48	1.25	1.26
45	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 133 and name CB)	13.67	1.26	1.27
	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 134 and name CA)	12.70	1.52	1.52
	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 135 and name CA)	13.51	0.96	0.96
	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 135 and name CB)	14.76	1.00	1.00
	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 136 and name CA)	11.61	1.30	1.30
	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 136 and name CB)	11.77	1.64	1.63
50	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 137 and name CA)	9.09	0.96	0.96
	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 138 and name CA)	10.35	1.34	1.34
	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 138 and name CB)	11.27	1.40	1.41
	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 139 and name CA)	12.50	0.90	0.89
	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 140 and name CA)	15.54	1.05	1.04
55	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 140 and name CB)	15.74	1.21	1.22
	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 141 and name CA)	18.32	0.86	0.87
	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 198 and name CA)	17.21	0.90	0.91
	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 198 and name CB)	16.58	0.96	0.96
60	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 201 and name CA)	16.86	0.71	0.72
	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 201 and name CB)	16.01	0.66	0.66
	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 202 and name CA)	15.36	0.83	0.83
	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 202 and name CB)	15.39	0.90	0.90
	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 205 and name CA)	15.17	0.95	0.94
65	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 205 and name CB)	13.89	0.92	0.92
	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 206 and name CA)	16.41	1.04	1.04
	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 206 and name CB)	17.05	1.04	1.03
	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 219 and name C)	6.88	0.35	0.36
	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 219 and name CA)	7.90	0.50	0.50
	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 219 and name CB)	9.08	0.45	0.46
70	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 219 and name O)	6.80	0.29	0.29
	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 220 and name C)	6.47	0.72	0.72
	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 220 and name CA)	5.66	0.52	0.52
	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 220 and name CB)	5.66	0.64	0.63
	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 220 and name N)	6.40	0.44	0.43
75	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 220 and name O)	6.17	0.94	0.94
	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 221 and name CA)	8.71	0.82	0.81
	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 221 and name CB)	10.02	0.77	0.77
	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 222 and name CA)	9.39	0.73	0.73
	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 222 and name CB)	9.74	0.59	0.59
80	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 223 and name CA)	6.61	0.99	0.99
	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 223 and name CB)	5.23	0.93	0.93
	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 224 and name CA)	7.74	1.44	1.45

	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 224 and name CB)	7.91	1.46	1.46
	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 225 and name CB)	11.15	1.35	1.34
	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 226 and name CB)	11.75	1.22	1.22
	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 240 and name CA)	11.37	1.31	1.32
	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 241 and name CA)	16.86	1.52	1.51
5	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 242 and name CA)	16.93	1.13	1.13
	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 243 and name CA)	18.00	1.04	1.03
	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 243 and name CB)	15.27	0.97	0.98
	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 244 and name CA)	15.05	1.06	1.06
	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 244 and name CB)	12.67	0.98	0.99
10	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 245 and name CA)	12.77	1.04	1.04
	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 245 and name CB)	14.89	0.87	0.87
	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 246 and name CA)	16.37	0.88	0.87
	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 246 and name CB)	15.31	0.84	0.84
	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 247 and name CA)	16.04	0.75	0.75
15	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 247 and name CB)	11.74	0.81	0.82
	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 248 and name CA)	10.69	0.89	0.88
	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 248 and name CB)	11.52	1.01	1.00
	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 249 and name CA)	11.95	1.09	1.08
	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 250 and name CA)	14.80	0.98	0.98
20	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 250 and name CB)	13.97	1.00	1.00
	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 251 and name CA)	13.67	0.98	0.98
	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 251 and name CB)	11.17	1.11	1.11
	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 252 and name CA)	9.86	1.12	1.12
	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 252 and name CB)	13.82	1.14	1.15
25	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 253 and name CA)	14.50	1.12	1.13
	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 254 and name CA)	16.68	1.15	1.15
	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 255 and name CA)	15.48	1.29	1.29
	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 256 and name CA)	14.34	1.03	1.04
	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 256 and name CB)	17.10	0.99	1.00
30	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 259 and name CB)	17.59	1.06	1.06
	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 388 and name CA)	17.64	0.75	0.74
	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 388 and name CB)	18.14	0.74	0.73
	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 389 and name CA)	16.74	0.51	0.50
	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 389 and name CB)	17.75	0.56	0.55
35	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 390 and name CA)	16.31	0.64	0.64
	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 390 and name CB)	16.48	0.64	0.64
	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 391 and name CA)	14.15	0.81	0.82
	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 391 and name CB)	14.75	0.86	0.86
	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 392 and name CA)	10.52	0.74	0.75
40	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 392 and name CB)	9.74	0.68	0.68
	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 393 and name CA)	10.55	1.00	0.99
	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 394 and name CA)	13.47	1.01	1.01
	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 394 and name CB)	14.13	0.94	0.94
	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 395 and name CA)	12.40	1.09	1.09
45	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 396 and name CA)	11.48	1.35	1.35
	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 396 and name CB)	10.41	1.33	1.33
	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 397 and name CA)	14.66	1.24	1.25
	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 397 and name CB)	15.06	1.15	1.15
	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 398 and name CA)	16.77	1.28	1.28
50	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 398 and name CB)	16.86	1.22	1.22
	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 399 and name CA)	15.89	1.43	1.44
	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 399 and name CB)	14.63	1.46	1.46
	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 400 and name CA)	16.77	1.46	1.46
	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 400 and name CB)	16.15	1.45	1.45
55	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 86 and name C)	5.74	0.12	0.12
	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 86 and name CA)	4.62	0.05	0.06
	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 86 and name CB)	5.29	0.08	0.08
	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 86 and name N)	3.35	0.08	0.07
	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 86 and name O)	6.82	0.21	0.20
60	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 94 and name CA)	10.84	0.76	0.77
	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 94 and name CB)	10.10	0.86	0.87
	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 95 and name CA)	14.08	0.67	0.68
	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 95 and name CB)	14.64	0.66	0.66
	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 96 and name CA)	15.90	1.16	1.17
65	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 96 and name CB)	15.86	1.52	1.53
	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 97 and name CA)	14.94	0.88	0.89
	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 97 and name CB)	13.77	0.92	0.91
	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 98 and name CA)	15.82	1.02	1.01
	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 98 and name CB)	15.41	1.26	1.25
70	assign (segid 3A4 and resid 85 and name CB) (segid 3A4 and resid 223 and name CB)	6.87	0.57	0.58
	assign (segid 3A4 and resid 85 and name N) (segid 3A4 and resid 85 and name C)	2.48	0.04	0.04
	assign (segid 3A4 and resid 85 and name N) (segid 3A4 and resid 85 and name CA)	1.45	0.01	0.01
	assign (segid 3A4 and resid 85 and name N) (segid 3A4 and resid 85 and name CB)	2.47	0.02	0.02
	assign (segid 3A4 and resid 85 and name N) (segid 3A4 and resid 85 and name O)	3.57	0.04	0.05
75	assign (segid 3A4 and resid 85 and name N) (segid 3A4 and resid 86 and name C)	4.80	0.11	0.11
	assign (segid 3A4 and resid 85 and name N) (segid 3A4 and resid 86 and name CA)	4.21	0.09	0.08
	assign (segid 3A4 and resid 85 and name N) (segid 3A4 and resid 86 and name CB)	5.01	0.14	0.15
	assign (segid 3A4 and resid 85 and name N) (segid 3A4 and resid 86 and name N)	2.78	0.08	0.08
	assign (segid 3A4 and resid 85 and name N) (segid 3A4 and resid 86 and name O)	5.90	0.30	0.31
80	assign (segid 3A4 and resid 85 and name N) (segid 3A4 and resid 85 and name CB)	3.14	0.11	0.11
	assign (segid 3A4 and resid 85 and name O) (segid 3A4 and resid 86 and name C)	3.55	0.21	0.20
	assign (segid 3A4 and resid 85 and name O) (segid 3A4 and resid 86 and name CA)	2.76	0.03	0.02

5	assign (segid 3A4 and resid 85 and name O) (segid 3A4 and resid 86 and name CB)	3.99	0.16	0.16
	assign (segid 3A4 and resid 85 and name O) (segid 3A4 and resid 86 and name N)	2.24	0.00	0.00
	assign (segid 3A4 and resid 85 and name O) (segid 3A4 and resid 86 and name O)	4.54	0.16	0.16
	assign (segid 3A4 and resid 85 and name O) (segid 3A4 and resid 94 and name CG)	6.43	0.73	0.73
	assign (segid 3A4 and resid 86 and name C) (segid 3A4 and resid 392 and name C)	6.33	0.65	0.64
	assign (segid 3A4 and resid 86 and name C) (segid 3A4 and resid 392 and name O)	5.25	0.66	0.65
	assign (segid 3A4 and resid 86 and name C) (segid 3A4 and resid 86 and name CB)	2.50	0.03	0.04
	assign (segid 3A4 and resid 86 and name C) (segid 3A4 and resid 86 and name O)	1.24	0.02	0.01
10	assign (segid 3A4 and resid 86 and name CA) (segid 3A4 and resid 100 and name CA)	18.43	0.92	0.92
	assign (segid 3A4 and resid 86 and name CA) (segid 3A4 and resid 100 and name CB)	18.07	1.18	1.19
	assign (segid 3A4 and resid 86 and name CA) (segid 3A4 and resid 101 and name CA)	17.91	0.77	0.78
	assign (segid 3A4 and resid 86 and name CA) (segid 3A4 and resid 101 and name CB)	16.77	0.73	0.73
	assign (segid 3A4 and resid 86 and name CA) (segid 3A4 and resid 102 and name CA)	19.24	0.28	0.28
	assign (segid 3A4 and resid 86 and name CA) (segid 3A4 and resid 129 and name CA)	17.14	1.19	1.20
15	assign (segid 3A4 and resid 86 and name CA) (segid 3A4 and resid 129 and name CB)	17.43	1.21	1.22
	assign (segid 3A4 and resid 86 and name CA) (segid 3A4 and resid 130 and name CA)	15.37	1.11	1.12
	assign (segid 3A4 and resid 86 and name CA) (segid 3A4 and resid 130 and name CB)	15.96	1.47	1.47
	assign (segid 3A4 and resid 86 and name CA) (segid 3A4 and resid 131 and name CA)	16.07	1.04	1.03
20	assign (segid 3A4 and resid 86 and name CA) (segid 3A4 and resid 131 and name CB)	17.36	1.06	1.06
	assign (segid 3A4 and resid 86 and name CA) (segid 3A4 and resid 132 and name CA)	15.20	1.42	1.43
	assign (segid 3A4 and resid 86 and name CA) (segid 3A4 and resid 132 and name CB)	15.77	1.84	1.84
	assign (segid 3A4 and resid 86 and name CA) (segid 3A4 and resid 133 and name CA)	12.34	0.98	0.97
	assign (segid 3A4 and resid 86 and name CA) (segid 3A4 and resid 133 and name CB)	12.15	0.87	0.87
25	assign (segid 3A4 and resid 86 and name CA) (segid 3A4 and resid 134 and name CA)	12.12	1.41	1.41
	assign (segid 3A4 and resid 86 and name CA) (segid 3A4 and resid 135 and name CA)	13.71	0.96	0.96
	assign (segid 3A4 and resid 86 and name CA) (segid 3A4 and resid 135 and name CB)	14.84	1.18	1.18
	assign (segid 3A4 and resid 86 and name CA) (segid 3A4 and resid 136 and name CA)	11.99	1.63	1.63
	assign (segid 3A4 and resid 86 and name CA) (segid 3A4 and resid 136 and name CB)	11.72	2.09	2.10
30	assign (segid 3A4 and resid 86 and name CA) (segid 3A4 and resid 137 and name CA)	9.84	0.70	0.71
	assign (segid 3A4 and resid 86 and name CA) (segid 3A4 and resid 138 and name CA)	11.95	1.24	1.23
	assign (segid 3A4 and resid 86 and name CA) (segid 3A4 and resid 138 and name CB)	12.64	1.36	1.36
	assign (segid 3A4 and resid 86 and name CA) (segid 3A4 and resid 139 and name CA)	14.32	0.91	0.91
	assign (segid 3A4 and resid 86 and name CA) (segid 3A4 and resid 140 and name CA)	16.91	0.98	0.99
35	assign (segid 3A4 and resid 86 and name CA) (segid 3A4 and resid 140 and name CB)	16.98	1.05	1.06
	assign (segid 3A4 and resid 86 and name CA) (segid 3A4 and resid 198 and name CB)	18.40	0.97	0.96
	assign (segid 3A4 and resid 86 and name CA) (segid 3A4 and resid 205 and name CB)	17.45	1.21	1.20
	assign (segid 3A4 and resid 86 and name CA) (segid 3A4 and resid 219 and name CA)	10.63	0.88	0.88
	assign (segid 3A4 and resid 86 and name CA) (segid 3A4 and resid 219 and name CB)	11.64	0.94	0.95
40	assign (segid 3A4 and resid 86 and name CA) (segid 3A4 and resid 220 and name CA)	8.54	0.97	0.97
	assign (segid 3A4 and resid 86 and name CA) (segid 3A4 and resid 220 and name CB)	7.84	0.95	0.96
	assign (segid 3A4 and resid 86 and name CA) (segid 3A4 and resid 221 and name CB)	11.93	1.16	1.16
	assign (segid 3A4 and resid 86 and name CA) (segid 3A4 and resid 221 and name CA)	13.03	1.15	1.15
	assign (segid 3A4 and resid 86 and name CA) (segid 3A4 and resid 222 and name CA)	13.35	1.05	1.05
45	assign (segid 3A4 and resid 86 and name CA) (segid 3A4 and resid 222 and name CB)	13.64	1.00	1.00
	assign (segid 3A4 and resid 86 and name CA) (segid 3A4 and resid 223 and name CA)	10.92	1.05	1.05
	assign (segid 3A4 and resid 86 and name CA) (segid 3A4 and resid 223 and name CB)	9.49	0.99	0.98
	assign (segid 3A4 and resid 86 and name CA) (segid 3A4 and resid 224 and name CA)	11.66	1.41	1.40
	assign (segid 3A4 and resid 86 and name CA) (segid 3A4 and resid 224 and name CB)	11.44	1.51	1.52
50	assign (segid 3A4 and resid 86 and name CA) (segid 3A4 and resid 225 and name CA)	15.24	1.35	1.35
	assign (segid 3A4 and resid 86 and name CA) (segid 3A4 and resid 225 and name CB)	15.84	1.30	1.29
	assign (segid 3A4 and resid 86 and name CA) (segid 3A4 and resid 226 and name CA)	15.79	1.22	1.22
	assign (segid 3A4 and resid 86 and name CA) (segid 3A4 and resid 243 and name CA)	17.44	0.98	0.97
	assign (segid 3A4 and resid 86 and name CA) (segid 3A4 and resid 243 and name CB)	17.30	1.05	1.04
55	assign (segid 3A4 and resid 86 and name CA) (segid 3A4 and resid 244 and name CA)	1		

	assign (segid 3A4 and resid 86 and name CA) (segid 3A4 and resid 386 and name CA)	17.32	0.95	0.94
	assign (segid 3A4 and resid 86 and name CA) (segid 3A4 and resid 387 and name CA)	17.21	1.10	1.10
	assign (segid 3A4 and resid 86 and name CA) (segid 3A4 and resid 388 and name CA)	15.34	0.93	0.93
	assign (segid 3A4 and resid 86 and name CA) (segid 3A4 and resid 388 and name CB)	16.16	0.91	0.91
5	assign (segid 3A4 and resid 86 and name CA) (segid 3A4 and resid 389 and name CA)	14.31	0.56	0.57
	assign (segid 3A4 and resid 86 and name CA) (segid 3A4 and resid 389 and name CB)	15.43	0.56	0.56
	assign (segid 3A4 and resid 86 and name CA) (segid 3A4 and resid 390 and name CA)	13.03	0.76	0.75
	assign (segid 3A4 and resid 86 and name CA) (segid 3A4 and resid 390 and name CB)	13.04	0.81	0.82
	assign (segid 3A4 and resid 86 and name CA) (segid 3A4 and resid 391 and name CA)	10.63	0.76	0.77
10	assign (segid 3A4 and resid 86 and name CA) (segid 3A4 and resid 391 and name CB)	11.03	0.78	0.78
	assign (segid 3A4 and resid 86 and name CA) (segid 3A4 and resid 392 and name C)	6.32	0.72	0.73
	assign (segid 3A4 and resid 86 and name CA) (segid 3A4 and resid 392 and name CA)	7.16	0.65	0.64
	assign (segid 3A4 and resid 86 and name CA) (segid 3A4 and resid 392 and name CB)	6.93	0.51	0.52
	assign (segid 3A4 and resid 86 and name CA) (segid 3A4 and resid 392 and name O)	5.41	0.78	0.77
15	assign (segid 3A4 and resid 86 and name CA) (segid 3A4 and resid 393 and name CA)	6.67	0.79	0.80
	assign (segid 3A4 and resid 86 and name CA) (segid 3A4 and resid 394 and name CA)	9.10	0.98	0.97
	assign (segid 3A4 and resid 86 and name CA) (segid 3A4 and resid 394 and name CB)	9.75	0.97	0.97
	assign (segid 3A4 and resid 86 and name CA) (segid 3A4 and resid 395 and name CA)	7.93	1.04	1.04
	assign (segid 3A4 and resid 86 and name CA) (segid 3A4 and resid 396 and name CA)	7.55	1.02	1.02
20	assign (segid 3A4 and resid 86 and name CA) (segid 3A4 and resid 396 and name CB)	6.71	0.95	0.95
	assign (segid 3A4 and resid 86 and name CA) (segid 3A4 and resid 397 and name CA)	10.70	0.96	0.96
	assign (segid 3A4 and resid 86 and name CA) (segid 3A4 and resid 397 and name CB)	11.04	0.91	0.92
	assign (segid 3A4 and resid 86 and name CA) (segid 3A4 and resid 398 and name CA)	12.53	1.08	1.08
	assign (segid 3A4 and resid 86 and name CA) (segid 3A4 and resid 398 and name CB)	12.50	1.09	1.08
25	assign (segid 3A4 and resid 86 and name CA) (segid 3A4 and resid 399 and name CA)	12.09	1.07	1.07
	assign (segid 3A4 and resid 86 and name CA) (segid 3A4 and resid 399 and name CB)	10.96	1.05	1.05
	assign (segid 3A4 and resid 86 and name CA) (segid 3A4 and resid 400 and name CA)	13.39	0.96	0.97
	assign (segid 3A4 and resid 86 and name CA) (segid 3A4 and resid 400 and name CB)	12.88	0.93	0.94
	assign (segid 3A4 and resid 86 and name CA) (segid 3A4 and resid 401 and name CA)	16.11	1.01	1.02
30	assign (segid 3A4 and resid 86 and name CA) (segid 3A4 and resid 402 and name CA)	17.23	1.11	1.11
	assign (segid 3A4 and resid 86 and name CA) (segid 3A4 and resid 402 and name CB)	16.61	1.16	1.17
	assign (segid 3A4 and resid 86 and name CA) (segid 3A4 and resid 403 and name CA)	17.42	0.98	0.98
	assign (segid 3A4 and resid 86 and name CA) (segid 3A4 and resid 403 and name CB)	16.38	0.95	0.94
	assign (segid 3A4 and resid 86 and name CA) (segid 3A4 and resid 86 and name C)	1.52	0.01	0.01
35	assign (segid 3A4 and resid 86 and name CA) (segid 3A4 and resid 86 and name CB)	1.52	0.01	0.02
	assign (segid 3A4 and resid 86 and name CA) (segid 3A4 and resid 86 and name O)	2.39	0.02	0.01
	assign (segid 3A4 and resid 86 and name CA) (segid 3A4 and resid 94 and name CA)	9.44	0.97	0.97
	assign (segid 3A4 and resid 86 and name CA) (segid 3A4 and resid 94 and name CB)	8.42	0.86	0.86
	assign (segid 3A4 and resid 86 and name CA) (segid 3A4 and resid 95 and name CA)	12.08	0.66	0.67
40	assign (segid 3A4 and resid 86 and name CA) (segid 3A4 and resid 95 and name CB)	12.53	0.61	0.61
	assign (segid 3A4 and resid 86 and name CA) (segid 3A4 and resid 96 and name CA)	14.70	1.39	1.38
	assign (segid 3A4 and resid 86 and name CA) (segid 3A4 and resid 96 and name CB)	15.01	1.74	1.74
	assign (segid 3A4 and resid 86 and name CA) (segid 3A4 and resid 97 and name CA)	13.94	1.17	1.16
	assign (segid 3A4 and resid 86 and name CA) (segid 3A4 and resid 97 and name CB)	12.93	1.24	1.24
45	assign (segid 3A4 and resid 86 and name CA) (segid 3A4 and resid 98 and name CA)	13.89	0.51	0.50
	assign (segid 3A4 and resid 86 and name CA) (segid 3A4 and resid 98 and name CB)	13.17	0.70	0.70
	assign (segid 3A4 and resid 86 and name CA) (segid 3A4 and resid 99 and name CA)	17.09	0.47	0.47
	assign (segid 3A4 and resid 86 and name CA) (segid 3A4 and resid 99 and name CB)	17.43	0.50	0.49
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 101 and name CA)	18.18	0.87	0.86
50	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 101 and name CB)	16.97	0.81	0.81
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 129 and name CA)	16.79	1.32	1.32
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 129 and name CB)	17.05	1.35	1.36
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 130 and name CA)	14.87	1.19	1.19
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 130 and name CB)	15.36	1.54	1.55
55	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 131 and name CA)	15.62	1.19	1.20
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 131 and name CB)	16.91	1.22	1.22
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 132 and name CA)	15.03	1.48	1.47
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 132 and name CB)	15.62	1.90	1.91
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 133 and name CA)	12.16	1.12	1.13
60	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 133 and name CB)	11.91	1.02	1.03
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 134 and name CA)	11.78	1.52	1.52
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 135 and name CA)	13.58	1.02	1.03
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 135 and name CB)	14.72	1.19	1.19
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 136 and name CA)	12.18	1.62	1.61
65	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 136 and name CB)	11.95	2.13	2.13
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 137 and name CA)	9.95	0.70	0.70
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 138 and name CA)	11.87	1.34	1.35
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 138 and name CB)	12.40	1.50	1.50
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 139 and name CA)	14.50	0.96	0.96
70	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 140 and name CA)	16.85	1.09	1.10
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 140 and name CB)	16.82	1.21	1.22
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 198 and name CA)	17.70	1.04	1.03
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 201 and name CB)	18.22	1.02	1.03
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 202 and name CA)	18.31	1.13	1.14
75	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 202 and name CB)	18.16	1.14	1.14
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 205 and name CA)	17.56	1.23	1.23
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 219 and name CA)	11.19	0.81	0.80
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 219 and name CB)	12.07	0.90	0.90
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 220 and name CA)	8.75	0.89	0.90
80	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 220 and name CB)	7.86	0.91	0.90
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 221 and name CA)	11.91	1.16	1.16
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 221 and name CB)	12.95	1.17	1.18
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 222 and name CA)	13.70	0.99	0.98

	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 222 and name CB)	14.12	0.93	0.93
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 223 and name CB)	11.38	0.92	0.93
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 223 and name CB)	10.01	0.84	0.85
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 224 and name CB)	11.66	1.34	1.33
5	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 224 and name CB)	11.27	1.48	1.47
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 225 and name CB)	15.29	1.30	1.31
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 225 and name CB)	15.92	1.25	1.26
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 226 and name CB)	16.14	1.14	1.14
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 226 and name CB)	16.62	0.97	0.97
10	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 243 and name CB)	16.52	1.02	1.03
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 244 and name CB)	14.64	0.99	0.99
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 244 and name CB)	15.21	1.02	1.01
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 245 and name CB)	16.17	0.91	0.92
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 245 and name CB)	17.69	0.91	0.91
15	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 246 and name CB)	15.51	0.75	0.74
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 246 and name CB)	16.17	0.66	0.66
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 247 and name CB)	11.78	0.76	0.77
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 247 and name CB)	11.15	0.86	0.86
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 248 and name CB)	11.88	0.95	0.95
20	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 248 and name CB)	12.83	1.02	1.02
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 249 and name CB)	14.22	0.83	0.83
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 250 and name CB)	12.29	0.74	0.74
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 250 and name CB)	11.99	0.66	0.67
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 251 and name CB)	9.30	0.84	0.84
25	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 251 and name CB)	8.50	0.84	0.85
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 252 and name CB)	12.19	0.91	0.92
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 252 and name CB)	13.32	0.91	0.91
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 253 and name CB)	14.26	0.99	0.99
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 254 and name CB)	12.10	1.16	1.16
30	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 255 and name CB)	10.89	0.96	0.97
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 256 and name CB)	14.07	0.75	0.74
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 257 and name CB)	16.65	1.04	1.03
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 258 and name CB)	15.42	1.03	1.02
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 258 and name CB)	14.32	1.11	1.11
35	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 259 and name CB)	14.67	0.81	0.82
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 259 and name CB)	13.63	0.80	0.81
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 260 and name CB)	17.91	0.96	0.95
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 260 and name CB)	18.36	1.11	1.12
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 262 and name CB)	17.42	0.73	0.73
40	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 318 and name CB)	18.96	0.47	0.46
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 319 and name CB)	17.50	1.04	1.04
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 383 and name CB)	17.11	0.89	0.89
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 384 and name CB)	13.63	0.88	0.89
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 384 and name CB)	12.65	1.03	1.04
45	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 385 and name CB)	15.45	0.80	0.81
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 386 and name CB)	16.29	1.00	0.99
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 387 and name CB)	16.23	1.19	1.18
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 388 and name CB)	14.35	1.06	1.06
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 388 and name CB)	15.18	1.03	1.04
50	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 389 and name CB)	13.09	0.63	0.62
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 389 and name CB)	14.15	0.59	0.58
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 390 and name CB)	11.90	0.82	0.81
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 390 and name CB)	12.04	0.91	0.91
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 391 and name CB)	9.40	0.78	0.78
55	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 391 and name CB)	9.83	0.78	0.78
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 392 and name CB)	5.14	0.78	0.78
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 392 and name CB)	5.93	0.71	0.70
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 392 and name CB)	5.64	0.48	0.47
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 392 and name CB)	4.38	0.88	0.88
60	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 393 and name CB)	5.60	0.78	0.79
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 393 and name CB)	5.71	0.75	0.76
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 394 and name CB)	8.36	0.95	0.95
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 394 and name CB)	9.01	0.97	0.98
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 395 and name CB)	7.84	0.96	0.96
65	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 396 and name CB)	7.44	0.91	0.91
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 396 and name CB)	6.50	0.87	0.86
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 397 and name CB)	10.19	0.89	0.89
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 397 and name CB)	10.36	0.86	0.86
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 398 and name CB)	12.31	0.97	0.97
70	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 398 and name CB)	12.31	0.98	0.99
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 399 and name CB)	12.26	0.91	0.91
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 399 and name CB)	11.26	0.88	0.88
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 400 and name CB)	13.34	0.84	0.84
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 400 and name CB)	12.71	0.82	0.82
75	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 401 and name CB)	15.89	0.90	0.90
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 402 and name CB)	17.23	0.96	0.96
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 402 and name CB)	16.74	1.00	1.01
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 403 and name CB)	17.66	0.86	0.85
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 403 and name CB)	16.66	0.87	0.82
80	assign (segid 3A4 and resid 86 and name CB) (segid HEM and resid 1 and name CAC)	7.08	0.97	0.96
	assign (segid 3A4 and resid 86 and name CB) (segid HEM and resid 1 and name CBC)	6.63	0.67	0.66
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 94 and name CA)	10.36	1.11	1.10
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 94 and name CB)	9.22	0.99	1.00

	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 95 and name CA)	12.97	0.78	0.78
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 95 and name CB)	13.48	0.71	0.71
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 96 and name CA)	15.64	1.41	1.42
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 96 and name CB)	16.04	1.74	1.75
5	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 97 and name CA)	14.63	1.26	1.26
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 97 and name CB)	13.59	1.34	1.33
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 98 and name CA)	14.37	0.64	0.64
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 98 and name CB)	13.65	0.80	0.81
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 99 and name CA)	17.68	0.58	0.59
	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 99 and name CB)	18.12	0.62	0.61
10	assign (segid 3A4 and resid 86 and name CB) (segid 3A4 and resid 86 and name C)	2.47	0.04	0.04
	assign (segid 3A4 and resid 86 and name N) (segid 3A4 and resid 86 and name CA)	1.45	0.01	0.01
	assign (segid 3A4 and resid 86 and name N) (segid 3A4 and resid 86 and name CB)	2.45	0.04	0.03
	assign (segid 3A4 and resid 86 and name N) (segid 3A4 and resid 86 and name O)	3.55	0.14	0.14
15	assign (segid 3A4 and resid 86 and name O) (segid 3A4 and resid 392 and name C)	5.75	0.56	0.55
	assign (segid 3A4 and resid 86 and name O) (segid 3A4 and resid 392 and name CA)	6.71	0.49	0.50
	assign (segid 3A4 and resid 86 and name O) (segid 3A4 and resid 392 and name O)	4.65	0.58	0.57
	assign (segid 3A4 and resid 86 and name O) (segid 3A4 and resid 393 and name CA)	6.07	0.72	0.72
	assign (segid 3A4 and resid 86 and name O) (segid 3A4 and resid 393 and name N)	6.41	0.62	0.61
20	assign (segid 3A4 and resid 86 and name O) (segid 3A4 and resid 86 and name CB)	2.86	0.06	0.07
	assign (segid 3A4 and resid 8 and name C) (segid 3A4 and resid 10 and name C)	4.62	0.11	0.12
	assign (segid 3A4 and resid 8 and name C) (segid 3A4 and resid 10 and name CA)	4.59	0.10	0.09
	assign (segid 3A4 and resid 8 and name C) (segid 3A4 and resid 10 and name CB)	5.40	0.07	0.07
	assign (segid 3A4 and resid 8 and name C) (segid 3A4 and resid 10 and name N)	3.40	0.07	0.07
25	assign (segid 3A4 and resid 8 and name C) (segid 3A4 and resid 10 and name O)	5.72	0.15	0.14
	assign (segid 3A4 and resid 8 and name C) (segid 3A4 and resid 11 and name C)	4.88	0.10	0.09
	assign (segid 3A4 and resid 8 and name C) (segid 3A4 and resid 11 and name CA)	4.52	0.08	0.08
	assign (segid 3A4 and resid 8 and name C) (segid 3A4 and resid 11 and name CB)	4.25	0.13	0.13
	assign (segid 3A4 and resid 8 and name C) (segid 3A4 and resid 11 and name N)	3.84	0.06	0.07
30	assign (segid 3A4 and resid 8 and name C) (segid 3A4 and resid 11 and name O)	6.05	0.06	0.06
	assign (segid 3A4 and resid 8 and name C) (segid 3A4 and resid 12 and name C)	6.39	0.30	0.30
	assign (segid 3A4 and resid 8 and name C) (segid 3A4 and resid 12 and name CA)	5.22	0.24	0.25
	assign (segid 3A4 and resid 8 and name C) (segid 3A4 and resid 12 and name CB)	4.97	0.40	0.40
	assign (segid 3A4 and resid 8 and name C) (segid 3A4 and resid 12 and name N)	4.26	0.20	0.21
35	assign (segid 3A4 and resid 8 and name C) (segid 3A4 and resid 13 and name N)	6.34	0.36	0.37
	assign (segid 3A4 and resid 8 and name C) (segid 3A4 and resid 8 and name CB)	2.49	0.02	0.01
	assign (segid 3A4 and resid 8 and name C) (segid 3A4 and resid 8 and name O)	1.23	0.01	0.01
	assign (segid 3A4 and resid 8 and name C) (segid 3A4 and resid 9 and name C)	3.10	0.09	0.08
	assign (segid 3A4 and resid 8 and name C) (segid 3A4 and resid 9 and name CA)	2.45	0.01	0.02
40	assign (segid 3A4 and resid 8 and name C) (segid 3A4 and resid 9 and name CB)	3.70	0.04	0.05
	assign (segid 3A4 and resid 8 and name C) (segid 3A4 and resid 9 and name N)	1.33	0.01	0.01
	assign (segid 3A4 and resid 8 and name C) (segid 3A4 and resid 9 and name O)	3.93	0.16	0.15
	assign (segid 3A4 and resid 8 and name C) (segid 3A4 and resid 10 and name C)	5.51	0.13	0.13
	assign (segid 3A4 and resid 8 and name CA) (segid 3A4 and resid 10 and name CA)	5.52	0.08	0.07
45	assign (segid 3A4 and resid 8 and name CA) (segid 3A4 and resid 10 and name CB)	6.01	0.06	0.06
	assign (segid 3A4 and resid 8 and name CA) (segid 3A4 and resid 10 and name N)	4.44	0.04	0.04
	assign (segid 3A4 and resid 8 and name CA) (segid 3A4 and resid 10 and name O)	6.64	0.15	0.15
	assign (segid 3A4 and resid 8 and name CA) (segid 3A4 and resid 11 and name C)	5.71	0.15	0.15
	assign (segid 3A4 and resid 8 and name CA) (segid 3A4 and resid 11 and name CA)	5.08	0.15	0.16
50	assign (segid 3A4 and resid 8 and name CA) (segid 3A4 and resid 11 and name CB)	4.41	0.20	0.19
	assign (segid 3A4 and resid 8 and name CA) (segid 3A4 and resid 11 and name N)	4.55	0.13	0.13
	assign (segid 3A4 and resid 8 and name CA) (segid 3A4 and resid 11 and name O)	6.83	0.15	0.15
	assign (segid 3A4 and resid 8 and name CA) (segid 3A4 and resid 12 and name C)	6.40	0.26	0.25
	assign (segid 3A4 and resid 8 and name CA) (segid 3A4 and resid 12 and name CB)	6.27	0.42	0.43
55	assign (segid 3A4 and resid 8 and name CA) (segid 3A4 and resid 12 and name N)	5.34	0.22	0.22
	assign (segid 3A4 and resid 8 and name CA) (segid 3A4 and resid 13 and name CA)	8.91	0.29	0.28
	assign (segid 3A4 and resid 8 and name CA) (segid 3A4 and resid 13 and name CB)	8.96	0.29	0.29
	assign (segid 3A4 and resid 8 and name CA) (segid 3A4 and resid 19 and name CA)	13.84	2.16	2.16
60	assign (segid 3A4 and resid 8 and name CA) (segid 3A4 and resid 19 and name CB)	14.89	2.18	2.17
	assign (segid 3A4 and resid 8 and name CA) (segid 3A4 and resid 20 and name CA)	15.48	1.95	1.94
	assign (segid 3A4 and resid 8 and name CA) (segid 3A4 and resid 20 and name CB)	16.88	1.94	1.95
	assign (segid 3A4 and resid 8 and name CA) (segid 3A4 and resid 21 and name CA)	15.25	1.83	1.83
	assign (segid 3A4 and resid 8 and name CA) (segid 3A4 and resid 21 and name CB)	11.17	1.78	1.78
	assign (segid 3A4 and resid 8 and name CA) (segid 3A4 and resid 22 and name CA)	16.76	1.85	1.85
65	assign (segid 3A4 and resid 8 and name CA) (segid 3A4 and resid 23 and name CA)	15.47	1.63	1.63
	assign (segid 3A4 and resid 8 and name CA) (segid 3A4 and resid 23 and name CB)	14.24	1.62	1.61
	assign (segid 3A4 and resid 8 and name CA) (segid 3A4 and resid 25 and name CA)	17.87	1.11	1.11
	assign (segid 3A4 and resid 8 and name CA) (segid 3A4 and resid 312 and name CA)	17.85	1.55	1.56
	assign (segid 3A4 and resid 8 and name CA) (segid 3A4 and resid 313 and name CA)	17.27	1.30	1.31
70	assign (segid 3A4 and resid 8 and name CA) (segid 3A4 and resid 314 and name CA)	15.29	0.97	0.97
	assign (segid 3A4 and resid 8 and name CA) (segid 3A4 and resid 314 and name CB)	15.88	0.93	0.93
	assign (segid 3A4 and resid 8 and name CA) (segid 3A4 and resid 315 and name CA)	13.17	1.34	1.35
	assign (segid 3A4 and resid 8 and name CA) (segid 3A4 and resid 315 and name CB)	13.88	1.51	1.52
	assign (segid 3A4 and resid 8 and name CA) (segid 3A4 and resid 316 and name CA)	12.88	1.67	1.67
75	assign (segid 3A4 and resid 8 and name CA) (segid 3A4 and resid 317 and name CA)	13.13	1.24	1.23
	assign (segid 3A4 and resid 8 and name CA) (segid 3A4 and resid 318 and name CA)	14.56	1.85	1.85
	assign (segid 3A4 and resid 8 and name CA) (segid 3A4 and resid 318 and name CB)	15.81	2.04	2.05
	assign (segid 3A4 and resid 8 and name CA) (segid 3A4 and resid 319 and name CA)	15.03	1.80	1.80
	assign (segid 3A4 and resid 8 and name CA) (segid 3A4 and resid 319 and name CB)	16.27	1.71	1.71
80	assign (segid 3A4 and resid 8 and name CA) (segid 3A4 and resid 31 and name CA)	17.01	1.73	1.74
	assign (segid 3A4 and resid 8 and name CA) (segid 3A4 and resid 32 and name CA)	13.70	1.75	1.75
	assign (segid 3A4 and resid 8 and name CA) (segid 3A4 and resid 32 and name CB)	12.45	1.69	1.68
	assign (segid 3A4 and resid 8 and name CA) (segid 3A4 and resid 33 and name CA)	14.10	1.89	1.89

	assign (segid 3A4 and resid 8 and name CA) (segid 3A4 and resid 33 and name CB)	15.27	1.81	1.80
	assign (segid 3A4 and resid 8 and name CA) (segid 3A4 and resid 344 and name CA)	15.59	1.72	1.72
	assign (segid 3A4 and resid 8 and name CA) (segid 3A4 and resid 344 and name CB)	14.70	1.64	1.63
	assign (segid 3A4 and resid 8 and name CA) (segid 3A4 and resid 345 and name CA)	14.76	1.86	1.86
	assign (segid 3A4 and resid 8 and name CA) (segid 3A4 and resid 345 and name CB)	15.95	1.90	1.89
5	assign (segid 3A4 and resid 8 and name CA) (segid 3A4 and resid 346 and name CA)	11.52	1.68	1.67
	assign (segid 3A4 and resid 8 and name CA) (segid 3A4 and resid 346 and name CB)	10.37	1.63	1.62
	assign (segid 3A4 and resid 8 and name CA) (segid 3A4 and resid 347 and name CA)	12.92	1.42	1.42
	assign (segid 3A4 and resid 8 and name CA) (segid 3A4 and resid 347 and name CB)	13.89	1.45	1.45
10	assign (segid 3A4 and resid 8 and name CA) (segid 3A4 and resid 348 and name CA)	10.14	1.00	1.00
	assign (segid 3A4 and resid 8 and name CA) (segid 3A4 and resid 349 and name CA)	9.09	1.25	1.25
	assign (segid 3A4 and resid 8 and name CA) (segid 3A4 and resid 349 and name CB)	8.93	1.49	1.49
	assign (segid 3A4 and resid 8 and name CA) (segid 3A4 and resid 34 and name CA)	11.45	1.91	1.91
	assign (segid 3A4 and resid 8 and name CA) (segid 3A4 and resid 34 and name CB)	10.54	2.09	2.09
	assign (segid 3A4 and resid 8 and name CA) (segid 3A4 and resid 350 and name CA)	12.43	1.31	1.31
15	assign (segid 3A4 and resid 8 and name CA) (segid 3A4 and resid 350 and name CB)	13.52	1.31	1.31
	assign (segid 3A4 and resid 8 and name CA) (segid 3A4 and resid 351 and name CA)	12.80	0.86	0.86
	assign (segid 3A4 and resid 8 and name CA) (segid 3A4 and resid 352 and name CA)	10.58	1.27	1.27
	assign (segid 3A4 and resid 8 and name CA) (segid 3A4 and resid 352 and name CB)	9.28	1.23	1.23
20	assign (segid 3A4 and resid 8 and name CA) (segid 3A4 and resid 353 and name CA)	12.27	1.71	1.70
	assign (segid 3A4 and resid 8 and name CA) (segid 3A4 and resid 353 and name CB)	13.19	1.74	1.74
	assign (segid 3A4 and resid 8 and name CA) (segid 3A4 and resid 354 and name CA)	13.93	1.88	1.88
	assign (segid 3A4 and resid 8 and name CA) (segid 3A4 and resid 354 and name CB)	13.66	1.98	1.98
	assign (segid 3A4 and resid 8 and name CA) (segid 3A4 and resid 357 and name CA)	15.67	1.44	1.44
25	assign (segid 3A4 and resid 8 and name CA) (segid 3A4 and resid 359 and name CA)	15.24	2.01	2.00
	assign (segid 3A4 and resid 8 and name CA) (segid 3A4 and resid 35 and name CA)	13.70	1.86	1.85
	assign (segid 3A4 and resid 8 and name CA) (segid 3A4 and resid 360 and name CA)	12.85	1.67	1.67
	assign (segid 3A4 and resid 8 and name CA) (segid 3A4 and resid 360 and name CB)	12.11	1.66	1.67
30	assign (segid 3A4 and resid 8 and name CA) (segid 3A4 and resid 361 and name CA)	11.36	1.82	1.82
	assign (segid 3A4 and resid 8 and name CA) (segid 3A4 and resid 361 and name CB)	10.58	1.99	2.00
	assign (segid 3A4 and resid 8 and name CA) (segid 3A4 and resid 362 and name CA)	14.91	1.77	1.76
	assign (segid 3A4 and resid 8 and name CA) (segid 3A4 and resid 362 and name CB)	15.98	1.83	1.82
	assign (segid 3A4 and resid 8 and name CA) (segid 3A4 and resid 363 and name CA)	16.73	1.58	1.58
	assign (segid 3A4 and resid 8 and name CA) (segid 3A4 and resid 363 and name CB)	16.88	1.66	1.66
35	assign (segid 3A4 and resid 8 and name CA) (segid 3A4 and resid 36 and name CA)	15.72	1.78	1.77
	assign (segid 3A4 and resid 8 and name CA) (segid 3A4 and resid 381 and name CA)	17.90	1.06	1.06
	assign (segid 3A4 and resid 8 and name CA) (segid 3A4 and resid 382 and name CA)	17.59	0.99	1.00
	assign (segid 3A4 and resid 8 and name CA) (segid 3A4 and resid 382 and name CB)	17.13	1.10	1.10
	assign (segid 3A4 and resid 8 and name CA) (segid 3A4 and resid 383 and name CA)	17.07	1.03	1.02
40	assign (segid 3A4 and resid 8 and name CA) (segid 3A4 and resid 38 and name CB)	17.33	1.96	1.96
	assign (segid 3A4 and resid 8 and name CA) (segid 3A4 and resid 39 and name CA)	17.32	1.73	1.73
	assign (segid 3A4 and resid 8 and name CA) (segid 3A4 and resid 39 and name CB)	16.18	1.63	1.64
	assign (segid 3A4 and resid 8 and name CA) (segid 3A4 and resid 427 and name CA)	14.28	3.33	3.32
	assign (segid 3A4 and resid 8 and name CA) (segid 3A4 and resid 428 and name CA)	13.89	2.61	2.61
45	assign (segid 3A4 and resid 8 and name CA) (segid 3A4 and resid 429 and name CA)	13.69	2.40	2.39
	assign (segid 3A4 and resid 8 and name CA) (segid 3A4 and resid 430 and name CA)	13.94	1.03	1.03
	assign (segid 3A4 and resid 8 and name CA) (segid 3A4 and resid 431 and name CA)	15.58	1.91	1.90
	assign (segid 3A4 and resid 8 and name CA) (segid 3A4 and resid 433 and name CA)	13.77	2.15	2.14
	assign (segid 3A4 and resid 8 and name CA) (segid 3A4 and resid 434 and name CA)	15.68	1.86	1.85
50	assign (segid 3A4 and resid 8 and name C)	1.52	0.01	0.01
	assign (segid 3A4 and resid 8 and name CB)	1.53	0.01	0.01
	assign (segid 3A4 and resid 8 and name O)	2.38	0.03	0.02
	assign (segid 3A4 and resid 9 and name C)	4.44	0.07	0.07
	assign (segid 3A4 and resid 9 and name CA)	3.81	0.01	0.02
55	assign (segid 3A4 and resid 9 and name CB)	4.85	0.04	0.04
	assign (segid 3A4 and resid 9 and name N)	2.44	0.01	0.01
	assign (segid 3A4 and resid 9 and name O)	5.35	0.14	0.14
	assign (segid 3A4 and resid 10 and name C)	6.93	0.13	0.13
60	assign (segid 3A4 and resid 10 and name CA)	6.88	0.05	0.05
	assign (segid 3A4 and resid 10 and name CB)	7.43	0.06	0.06
	assign (segid 3A4 and resid 10 and name N)	5.68	0.02	0.02
	assign (segid 3A4 and resid 11 and name C)	6.87	0.18	0.18
	assign (segid 3A4 and resid 11 and name CA)	6.43	0.19	0.19
	assign (segid 3A4 and resid 11 and name CB)	5.65	0.24	0.25
65	assign (segid 3A4 and resid 11 and name N)	5.98	0.13	0.14
	assign (segid 3A4 and resid 12 and name CA)	7.22	0.30	0.30
	assign (segid 3A4 and resid 12 and name CB)	6.87	0.49	0.48
	assign (segid 3A4 and resid 12 and name N)	6.36	0.24	0.25
	assign (segid 3A4 and resid 13 and name CA)	10.01	0.34	0.33
70	assign (segid 3A4 and resid 13 and name CB)	10.12	0.37	0.36
	assign (segid 3A4 and resid 19 and name CA)	15.09	2.34	2.34
	assign (segid 3A4 and resid 19 and name CB)	16.12	2.38	2.38
	assign (segid 3A4 and resid 20 and name CA)	16.72	2.16	2.17
	assign (segid 3A4 and resid 21 and name CA)	16.43	1.93	1.93
75	assign (segid 3A4 and resid 21 and name CB)	15.34	1.82	1.82
	assign (segid 3A4 and resid 23 and name CA)	16.40	1.70	1.69
	assign (segid 3A4 and resid 23 and name CB)	15.15	1.71	1.70
	assign (segid 3A4 and resid 265 and name CA)	17.46	2.28	2.28
	assign (segid 3A4 and resid 314 and name CA)	15.65	1.27	1.26
80	assign (segid 3A4 and resid 314 and name CB)	16.24	1.22	1.22
	assign (segid 3A4 and resid 315 and name CA)	13.33	1.38	1.37
	assign (segid 3A4 and resid 315 and name CB)	13.93	1.51	1.51
	assign (segid 3A4 and resid 316 and name CA)	12.95	1.66	1.66

	assign (segid 3A4 and resid 8 and name CB) (segid 3A4 and resid 317 and name CA)	13.45	1.52	1.52
	assign (segid 3A4 and resid 8 and name CB) (segid 3A4 and resid 318 and name CA)	14.79	1.95	1.95
	assign (segid 3A4 and resid 8 and name CB) (segid 3A4 and resid 318 and name CB)	15.99	2.13	2.14
	assign (segid 3A4 and resid 8 and name CB) (segid 3A4 and resid 319 and name CA)	15.47	2.01	2.02
5	assign (segid 3A4 and resid 8 and name CB) (segid 3A4 and resid 32 and name CA)	14.85	2.05	2.06
	assign (segid 3A4 and resid 8 and name CB) (segid 3A4 and resid 32 and name CB)	13.58	1.94	1.95
	assign (segid 3A4 and resid 8 and name CB) (segid 3A4 and resid 33 and name CA)	15.29	2.32	2.32
	assign (segid 3A4 and resid 8 and name CB) (segid 3A4 and resid 33 and name CB)	16.45	2.26	2.26
	assign (segid 3A4 and resid 8 and name CB) (segid 3A4 and resid 344 and name CA)	16.59	2.09	2.09
10	assign (segid 3A4 and resid 8 and name CB) (segid 3A4 and resid 344 and name CB)	15.66	1.97	1.97
	assign (segid 3A4 and resid 8 and name CB) (segid 3A4 and resid 345 and name CA)	15.78	2.35	2.35
	assign (segid 3A4 and resid 8 and name CB) (segid 3A4 and resid 345 and name CB)	16.96	2.40	2.40
	assign (segid 3A4 and resid 8 and name CB) (segid 3A4 and resid 346 and name CA)	12.48	2.22	2.21
	assign (segid 3A4 and resid 8 and name CB) (segid 3A4 and resid 346 and name CB)	11.37	2.20	2.19
15	assign (segid 3A4 and resid 8 and name CB) (segid 3A4 and resid 347 and name CA)	13.74	2.05	2.05
	assign (segid 3A4 and resid 8 and name CB) (segid 3A4 and resid 347 and name CB)	14.65	2.02	2.02
	assign (segid 3A4 and resid 8 and name CB) (segid 3A4 and resid 348 and name CA)	10.81	1.66	1.67
	assign (segid 3A4 and resid 8 and name CB) (segid 3A4 and resid 349 and name CA)	9.97	2.05	2.05
	assign (segid 3A4 and resid 8 and name CB) (segid 3A4 and resid 349 and name CB)	9.89	2.25	2.26
20	assign (segid 3A4 and resid 8 and name CB) (segid 3A4 and resid 34 and name CA)	12.61	2.39	2.39
	assign (segid 3A4 and resid 8 and name CB) (segid 3A4 and resid 34 and name CB)	11.73	2.48	2.47
	assign (segid 3A4 and resid 8 and name CB) (segid 3A4 and resid 350 and name CA)	13.34	2.03	2.02
	assign (segid 3A4 and resid 8 and name CB) (segid 3A4 and resid 350 and name CB)	14.43	2.04	2.04
	assign (segid 3A4 and resid 8 and name CB) (segid 3A4 and resid 351 and name CA)	13.48	1.54	1.53
25	assign (segid 3A4 and resid 8 and name CB) (segid 3A4 and resid 352 and name CA)	11.25	1.58	1.58
	assign (segid 3A4 and resid 8 and name CB) (segid 3A4 and resid 352 and name CB)	9.94	1.50	1.50
	assign (segid 3A4 and resid 8 and name CB) (segid 3A4 and resid 353 and name CA)	13.12	2.02	2.01
	assign (segid 3A4 and resid 8 and name CB) (segid 3A4 and resid 353 and name CB)	14.08	2.11	2.12
	assign (segid 3A4 and resid 8 and name CB) (segid 3A4 and resid 354 and name CA)	14.65	1.99	1.99
30	assign (segid 3A4 and resid 8 and name CB) (segid 3A4 and resid 354 and name CB)	14.36	2.03	2.03
	assign (segid 3A4 and resid 8 and name CB) (segid 3A4 and resid 357 and name CB)	16.22	1.61	1.61
	assign (segid 3A4 and resid 8 and name CB) (segid 3A4 and resid 359 and name CA)	15.46	1.89	1.89
	assign (segid 3A4 and resid 8 and name CB) (segid 3A4 and resid 35 and name CA)	14.83	2.32	2.32
	assign (segid 3A4 and resid 8 and name CB) (segid 3A4 and resid 360 and name CA)	13.20	1.61	1.61
35	assign (segid 3A4 and resid 8 and name CB) (segid 3A4 and resid 360 and name CB)	12.58	1.66	1.65
	assign (segid 3A4 and resid 8 and name CB) (segid 3A4 and resid 361 and name CA)	11.41	1.67	1.67
	assign (segid 3A4 and resid 8 and name CB) (segid 3A4 and resid 361 and name CB)	10.57	1.87	1.87
	assign (segid 3A4 and resid 8 and name CB) (segid 3A4 and resid 362 and name CA)	14.81	1.64	1.64
	assign (segid 3A4 and resid 8 and name CB) (segid 3A4 and resid 362 and name CB)	15.89	1.73	1.72
40	assign (segid 3A4 and resid 8 and name CB) (segid 3A4 and resid 363 and name CA)	16.60	1.46	1.47
	assign (segid 3A4 and resid 8 and name CB) (segid 3A4 and resid 363 and name CB)	16.67	1.54	1.55
	assign (segid 3A4 and resid 8 and name CB) (segid 3A4 and resid 382 and name CB)	17.93	1.87	1.87
	assign (segid 3A4 and resid 8 and name CB) (segid 3A4 and resid 39 and name CB)	17.23	2.29	2.30
	assign (segid 3A4 and resid 8 and name CB) (segid 3A4 and resid 426 and name CA)	13.99	2.74	2.75
45	assign (segid 3A4 and resid 8 and name CB) (segid 3A4 and resid 427 and name CA)	13.74	3.54	3.54
	assign (segid 3A4 and resid 8 and name CB) (segid 3A4 and resid 428 and name CA)	13.55	2.75	2.75
	assign (segid 3A4 and resid 8 and name CB) (segid 3A4 and resid 429 and name CA)	13.65	2.53	2.54
	assign (segid 3A4 and resid 8 and name CB) (segid 3A4 and resid 430 and name CA)	14.16	1.33	1.33
	assign (segid 3A4 and resid 8 and name CB) (segid 3A4 and resid 431 and name CA)	15.94	2.18	2.17
50	assign (segid 3A4 and resid 8 and name CB) (segid 3A4 and resid 433 and name CA)	13.73	2.33	2.33
	assign (segid 3A4 and resid 8 and name CB) (segid 3A4 and resid 434 and name CA)	15.42	1.89	1.89
	assign (segid 3A4 and resid 8 and name CB) (segid 3A4 and resid 9 and name C)	5.48	0.06	0.06
	assign (segid 3A4 and resid 8 and name CB) (segid 3A4 and resid 9 and name CB)	4.51	0.04	0.04
	assign (segid 3A4 and resid 8 and name CB) (segid 3A4 and resid 9 and name N)	5.34	0.10	0.10
55	assign (segid 3A4 and resid 8 and name CB) (segid 3A4 and resid 9 and name O)	6.35	0.15	0.14
	assign (segid 3A4 and resid 8 and name CB) (segid 3A4 and resid 10 and name C)	5.60	0.07	0.07
	assign (segid 3A4 and resid 8 and name N) (segid 3A4 and resid 10 and name CA)	5.36	0.09	0.08
	assign (segid 3A4 and resid 8 and name N) (segid 3A4 and resid 10 and name CB)	5.50	0.14	0.14
60	assign (segid 3A4 and resid 8 and name N) (segid 3A4 and resid 10 and name N)	4.33	0.10	0.11
	assign (segid 3A4 and resid 8 and name N) (segid 3A4 and resid 10 and name O)	6.80	0.07	0.08
	assign (segid 3A4 and resid 8 and name N) (segid 3A4 and resid 11 and name C)	6.45	0.10	0.09
	assign (segid 3A4 and resid 8 and name N) (segid 3A4 and resid 11 and name CA)	5.55	0.11	0.12
	assign (segid 3A4 and resid 8 and name N) (segid 3A4 and resid 11 and name CB)	4.97	0.15	0.15
65	assign (segid 3A4 and resid 8 and name N) (segid 3A4 and resid 11 and name N)	4.78	0.08	0.09
	assign (segid 3A4 and resid 8 and name N) (segid 3A4 and resid 11 and name O)	7.59	0.08	0.09
	assign (segid 3A4 and resid 8 and name N) (segid 3A4 and resid 12 and name CA)	7.39	0.21	0.22
	assign (segid 3A4 and resid 8 and name N) (segid 3A4 and resid 12 and name N)	6.21	0.18	0.18
	assign (segid 3A4 and resid 8 and name N) (segid 3A4 and resid 12 and name O)	2.47	0.03	0.02
70	assign (segid 3A4 and resid 8 and name N) (segid 3A4 and resid 8 and name CA)	1.46	0.00	0.01
	assign (segid 3A4 and resid 8 and name N) (segid 3A4 and resid 8 and name CB)	2.44	0.02	0.03
	assign (segid 3A4 and resid 8 and name N) (segid 3A4 and resid 8 and name O)	3.52	0.04	0.03
	assign (segid 3A4 and resid 8 and name N) (segid 3A4 and resid 9 and name C)	4.70	0.08	0.08
	assign (segid 3A4 and resid 8 and name N) (segid 3A4 and resid 9 and name CA)	4.20	0.08	0.08
75	assign (segid 3A4 and resid 8 and name N) (segid 3A4 and resid 9 and name CB)	4.96	0.08	0.09
	assign (segid 3A4 and resid 8 and name N) (segid 3A4 and resid 9 and name O)	2.80	0.08	0.08
	assign (segid 3A4 and resid 8 and name N) (segid 3A4 and resid 10 and name C)	1.31	0.24	0.24
	assign (segid 3A4 and resid 8 and name O) (segid 3A4 and resid 10 and name CA)	4.61	0.23	0.23
80	assign (segid 3A4 and resid 8 and name O) (segid 3A4 and resid 10 and name CB)	5.64	0.18	0.18
	assign (segid 3A4 and resid 8 and name O) (segid 3A4 and resid 10 and name N)	3.65	0.17	0.16
	assign (segid 3A4 and resid 8 and name O) (segid 3A4 and resid 10 and name O)	5.25	0.29	0.28
	assign (segid 3A4 and resid 8 and name O) (segid 3A4 and resid 11 and name C)	3.91	0.13	0.14

	assign	(segid 3A4 and resid 8 and name O)	(segid 3A4 and resid 11 and name CA)	3.84	0.13	0.14
	assign	(segid 3A4 and resid 8 and name O)	(segid 3A4 and resid 11 and name CB)	3.63	0.15	0.15
	assign	(segid 3A4 and resid 8 and name O)	(segid 3A4 and resid 11 and name N)	3.45	0.15	0.16
	assign	(segid 3A4 and resid 8 and name O)	(segid 3A4 and resid 11 and name O)	5.03	0.10	0.09
5	assign	(segid 3A4 and resid 8 and name O)	(segid 3A4 and resid 12 and name C)	5.37	0.31	0.31
	assign	(segid 3A4 and resid 8 and name O)	(segid 3A4 and resid 12 and name CA)	4.11	0.26	0.25
	assign	(segid 3A4 and resid 8 and name O)	(segid 3A4 and resid 12 and name CB)	3.95	0.39	0.39
	assign	(segid 3A4 and resid 8 and name O)	(segid 3A4 and resid 12 and name N)	3.21	0.24	0.24
	assign	(segid 3A4 and resid 8 and name O)	(segid 3A4 and resid 12 and name O)	6.45	0.29	0.28
10	assign	(segid 3A4 and resid 8 and name O)	(segid 3A4 and resid 13 and name CA)	6.86	0.38	0.38
	assign	(segid 3A4 and resid 8 and name O)	(segid 3A4 and resid 13 and name CB)	7.12	0.39	0.39
	assign	(segid 3A4 and resid 8 and name O)	(segid 3A4 and resid 13 and name N)	5.49	0.37	0.37
	assign	(segid 3A4 and resid 8 and name O)	(segid 3A4 and resid 13 and name O)	3.24	0.05	0.05
	assign	(segid 3A4 and resid 8 and name O)	(segid 3A4 and resid 9 and name C)	3.13	0.16	0.17
15	assign	(segid 3A4 and resid 8 and name O)	(segid 3A4 and resid 9 and name CB)	2.80	0.02	0.03
	assign	(segid 3A4 and resid 8 and name O)	(segid 3A4 and resid 9 and name N)	4.24	0.07	0.08
	assign	(segid 3A4 and resid 8 and name O)	(segid 3A4 and resid 9 and name O)	2.25	0.01	0.01
	assign	(segid 3A4 and resid 8 and name O)	(segid 3A4 and resid 9 and name O)	3.60	0.26	0.26
	assign	(segid 3A4 and resid 8 and name O)	(segid 3A4 and resid 9 and name O)	2.48	0.03	0.03
20	assign	(segid 3A4 and resid 94 and name C)	(segid 3A4 and resid 94 and name CB)	3.85	0.02	0.02
	assign	(segid 3A4 and resid 94 and name C)	(segid 3A4 and resid 94 and name O)	1.23	0.01	0.01
	assign	(segid 3A4 and resid 94 and name C)	(segid 3A4 and resid 95 and name C)	3.05	0.07	0.07
	assign	(segid 3A4 and resid 94 and name C)	(segid 3A4 and resid 95 and name CA)	2.44	0.02	0.01
	assign	(segid 3A4 and resid 94 and name C)	(segid 3A4 and resid 95 and name CB)	3.70	0.05	0.05
25	assign	(segid 3A4 and resid 94 and name C)	(segid 3A4 and resid 95 and name N)	1.31	0.01	0.02
	assign	(segid 3A4 and resid 94 and name C)	(segid 3A4 and resid 95 and name O)	3.90	0.10	0.10
	assign	(segid 3A4 and resid 94 and name C)	(segid 3A4 and resid 96 and name C)	4.59	0.10	0.11
	assign	(segid 3A4 and resid 94 and name C)	(segid 3A4 and resid 96 and name CA)	4.52	0.12	0.12
	assign	(segid 3A4 and resid 94 and name C)	(segid 3A4 and resid 96 and name CB)	5.23	0.11	0.12
30	assign	(segid 3A4 and resid 94 and name C)	(segid 3A4 and resid 96 and name N)	3.34	0.12	0.12
	assign	(segid 3A4 and resid 94 and name C)	(segid 3A4 and resid 96 and name O)	5.70	0.10	0.10
	assign	(segid 3A4 and resid 94 and name C)	(segid 3A4 and resid 97 and name C)	4.88	0.12	0.11
	assign	(segid 3A4 and resid 94 and name C)	(segid 3A4 and resid 97 and name CA)	4.52	0.14	0.14
	assign	(segid 3A4 and resid 94 and name C)	(segid 3A4 and resid 97 and name CB)	4.32	0.22	0.21
35	assign	(segid 3A4 and resid 94 and name C)	(segid 3A4 and resid 97 and name N)	3.82	0.14	0.14
	assign	(segid 3A4 and resid 94 and name C)	(segid 3A4 and resid 97 and name O)	6.06	0.10	0.10
	assign	(segid 3A4 and resid 94 and name C)	(segid 3A4 and resid 98 and name C)	6.27	0.33	0.32
	assign	(segid 3A4 and resid 94 and name C)	(segid 3A4 and resid 98 and name CA)	5.15	0.22	0.21
	assign	(segid 3A4 and resid 94 and name C)	(segid 3A4 and resid 98 and name CB)	4.86	0.35	0.35
40	assign	(segid 3A4 and resid 94 and name C)	(segid 3A4 and resid 98 and name N)	4.21	0.19	0.19
	assign	(segid 3A4 and resid 94 and name C)	(segid 3A4 and resid 98 and name O)	7.37	0.23	0.23
	assign	(segid 3A4 and resid 94 and name C)	(segid 3A4 and resid 99 and name N)	6.23	0.51	0.51
	assign	(segid 3A4 and resid 94 and name CA)	(segid 3A4 and resid 100 and name CA)	10.08	0.15	0.15
	assign	(segid 3A4 and resid 94 and name CA)	(segid 3A4 and resid 100 and name CB)	9.66	0.18	0.18
45	assign	(segid 3A4 and resid 94 and name CA)	(segid 3A4 and resid 101 and name CA)	10.73	0.40	0.40
	assign	(segid 3A4 and resid 94 and name CA)	(segid 3A4 and resid 101 and name CB)	10.00	0.54	0.54
	assign	(segid 3A4 and resid 94 and name CA)	(segid 3A4 and resid 102 and name CA)	12.35	0.10	0.10
	assign	(segid 3A4 and resid 94 and name CA)	(segid 3A4 and resid 103 and name CA)	14.43	0.06	0.06
	assign	(segid 3A4 and resid 94 and name CA)	(segid 3A4 and resid 103 and name CB)	14.15	0.09	0.09
50	assign	(segid 3A4 and resid 94 and name CA)	(segid 3A4 and resid 104 and name CA)	15.52	0.34	0.35
	assign	(segid 3A4 and resid 94 and name CA)	(segid 3A4 and resid 104 and name CB)	14.83	0.48	0.48
	assign	(segid 3A4 and resid 94 and name CA)	(segid 3A4 and resid 105 and name CA)	16.56	0.39	0.40
	assign	(segid 3A4 and resid 94 and name CA)	(segid 3A4 and resid 105 and name CB)	15.82	0.39	0.39
	assign	(segid 3A4 and resid 94 and name CA)	(segid 3A4 and resid 106 and name CA)	18.43	0.13	0.13
55	assign	(segid 3A4 and resid 94 and name CA)	(segid 3A4 and resid 106 and name CB)	18.00	0.14	0.13
	assign	(segid 3A4 and resid 94 and name CA)	(segid 3A4 and resid 107 and name CB)	19.60	0.17	0.17
	assign	(segid 3A4 and resid 94 and name CA)	(segid 3A4 and resid 126 and name CA)	18.62	0.34	0.33
	assign	(segid 3A4 and resid 94 and name CA)	(segid 3A4 and resid 127 and name CA)	18.50	0.88	0.88
	assign	(segid 3A4 and resid 94 and name CA)	(segid 3A4 and resid 128 and name CA)	16.18	1.30	1.31
60	assign	(segid 3A4 and resid 94 and name CA)	(segid 3A4 and resid 128 and name CB)	16.63	1.49	1.48
	assign	(segid 3A4 and resid 94 and name CA)	(segid 3A4 and resid 129 and name CA)	13.71	0.69	0.69
	assign	(segid 3A4 and resid 94 and name CA)	(segid 3A4 and resid 129 and name CB)	14.09	0.50	0.49
	assign	(segid 3A4 and resid 94 and name CA)	(segid 3A4 and resid 130 and name CA)	13.38	0.63	0.64
	assign	(segid 3A4 and resid 94 and name CA)	(segid 3A4 and resid 130 and name CB)	14.47	0.80	0.79
65	assign	(segid 3A4 and resid 94 and name CA)	(segid 3A4 and resid 131 and name CA)	13.85	0.92	0.93
	assign	(segid 3A4 and resid 94 and name CA)	(segid 3A4 and resid 131 and name CB)	14.97	1.28	1.29
	assign	(segid 3A4 and resid 94 and name CA)	(segid 3A4 and resid 132 and name CA)	11.61	1.65	1.65
	assign	(segid 3A4 and resid 94 and name CA)	(segid 3A4 and resid 132 and name CB)	11.69	1.84	1.83
	assign	(segid 3A4 and resid 94 and name CA)	(segid 3A4 and resid 133 and name CA)	9.56	0.50	0.50
70	assign	(segid 3A4 and resid 94 and name CA)	(segid 3A4 and resid 133 and name CB)	9.64	0.88	0.88
	assign	(segid 3A4 and resid 94 and name CA)	(segid 3A4 and resid 134 and name CA)	11.12	0.43	0.43
	assign	(segid 3A4 and resid 94 and name CA)	(segid 3A4 and resid 135 and name CA)	11.55	1.65	1.65
	assign	(segid 3A4 and resid 94 and name CA)	(segid 3A4 and resid 135 and name CB)	12.08	2.21	2.21
	assign	(segid 3A4 and resid 94 and name CA)	(segid 3A4 and resid 136 and name CA)	9.00	1.68	1.68
75	assign	(segid 3A4 and resid 94 and name CA)	(segid 3A4 and resid 136 and name CB)	8.17	1.68	1.68
	assign	(segid 3A4 and resid 94 and name CA)	(segid 3A4 and resid 137 and name CA)	9.13	0.69	0.70
	assign	(segid 3A4 and resid 94 and name CA)	(segid 3A4 and resid 138 and name CA)	12.24	0.53	0.53
	assign	(segid 3A4 and resid 94 and name CA)	(segid 3A4 and resid 138 and name CB)	13.24	0.52	0.52
	assign	(segid 3A4 and resid 94 and name CA)	(segid 3A4 and resid 139 and name CA)	12.56	1.31	1.31
80	assign	(segid 3A4 and resid 94 and name CA)	(segid 3A4 and resid 140 and name CA)	15.02	1.18	1.17
	assign	(segid 3A4 and resid 94 and name CA)	(segid 3A4 and resid 140 and name CB)	15.55	0.79	0.78
	assign	(segid 3A4 and resid 94 and name CA)	(segid 3A4 and resid 141 and name CA)	16.21	1.60	1.60
	assign	(segid 3A4 and resid 94 and name CA)	(segid 3A4 and resid 141 and name CB)	17.01	2.15	2.15

	assign (segid 3A4 and resid 94 and name CA) (segid 3A4 and resid 219 and name CA)	10.45	1.44	1.45
	assign (segid 3A4 and resid 94 and name CA) (segid 3A4 and resid 219 and name CB)	11.08	1.48	1.48
	assign (segid 3A4 and resid 94 and name CA) (segid 3A4 and resid 220 and name CA)	11.49	1.16	1.16
	assign (segid 3A4 and resid 94 and name CA) (segid 3A4 and resid 220 and name CB)	11.22	1.14	1.15
5	assign (segid 3A4 and resid 94 and name CA) (segid 3A4 and resid 221 and name CA)	14.86	1.21	1.22
	assign (segid 3A4 and resid 94 and name CA) (segid 3A4 and resid 221 and name CB)	15.36	1.21	1.21
	assign (segid 3A4 and resid 94 and name CA) (segid 3A4 and resid 222 and name CA)	15.55	1.35	1.34
	assign (segid 3A4 and resid 94 and name CA) (segid 3A4 and resid 222 and name CB)	14.99	1.37	1.38
	assign (segid 3A4 and resid 94 and name CA) (segid 3A4 and resid 223 and name CA)	14.76	1.22	1.21
10	assign (segid 3A4 and resid 94 and name CA) (segid 3A4 and resid 223 and name CB)	13.55	1.16	1.16
	assign (segid 3A4 and resid 94 and name CA) (segid 3A4 and resid 224 and name CA)	17.00	1.29	1.28
	assign (segid 3A4 and resid 94 and name CA) (segid 3A4 and resid 224 and name CB)	16.91	1.31	1.31
	assign (segid 3A4 and resid 94 and name CA) (segid 3A4 and resid 248 and name CA)	17.44	1.14	1.14
	assign (segid 3A4 and resid 94 and name CA) (segid 3A4 and resid 248 and name CB)	17.77	1.11	1.12
15	assign (segid 3A4 and resid 94 and name CA) (segid 3A4 and resid 251 and name CA)	15.38	0.99	1.00
	assign (segid 3A4 and resid 94 and name CA) (segid 3A4 and resid 251 and name CB)	14.46	1.03	1.03
	assign (segid 3A4 and resid 94 and name CA) (segid 3A4 and resid 252 and name CA)	16.19	0.82	0.82
	assign (segid 3A4 and resid 94 and name CA) (segid 3A4 and resid 252 and name CB)	17.04	0.81	0.81
	assign (segid 3A4 and resid 94 and name CA) (segid 3A4 and resid 255 and name CA)	14.87	1.45	1.46
20	assign (segid 3A4 and resid 94 and name CA) (segid 3A4 and resid 256 and name CA)	16.22	0.99	0.99
	assign (segid 3A4 and resid 94 and name CA) (segid 3A4 and resid 259 and name CA)	15.93	0.68	0.69
	assign (segid 3A4 and resid 94 and name CA) (segid 3A4 and resid 259 and name CB)	14.53	0.69	0.69
	assign (segid 3A4 and resid 94 and name CA) (segid 3A4 and resid 260 and name CA)	18.11	0.53	0.54
	assign (segid 3A4 and resid 94 and name CA) (segid 3A4 and resid 262 and name CB)	18.53	0.82	0.83
25	assign (segid 3A4 and resid 94 and name CA) (segid 3A4 and resid 263 and name CA)	18.81	0.35	0.34
	assign (segid 3A4 and resid 94 and name CA) (segid 3A4 and resid 263 and name CB)	17.86	0.29	0.28
	assign (segid 3A4 and resid 94 and name CA) (segid 3A4 and resid 306 and name CA)	17.93	0.98	0.98
	assign (segid 3A4 and resid 94 and name CA) (segid 3A4 and resid 309 and name CB)	17.46	0.75	0.76
	assign (segid 3A4 and resid 94 and name CA) (segid 3A4 and resid 384 and name CB)	18.58	1.07	1.07
30	assign (segid 3A4 and resid 94 and name CA) (segid 3A4 and resid 391 and name CA)	17.28	1.25	1.24
	assign (segid 3A4 and resid 94 and name CA) (segid 3A4 and resid 391 and name CB)	16.95	1.23	1.22
	assign (segid 3A4 and resid 94 and name CA) (segid 3A4 and resid 392 and name CA)	14.66	1.33	1.33
	assign (segid 3A4 and resid 94 and name CA) (segid 3A4 and resid 392 and name CB)	14.85	1.33	1.33
	assign (segid 3A4 and resid 94 and name CA) (segid 3A4 and resid 393 and name CA)	12.06	1.24	1.24
35	assign (segid 3A4 and resid 94 and name CA) (segid 3A4 and resid 394 and name CA)	13.29	1.24	1.24
	assign (segid 3A4 and resid 94 and name CA) (segid 3A4 and resid 394 and name CB)	14.40	1.32	1.32
	assign (segid 3A4 and resid 94 and name CA) (segid 3A4 and resid 395 and name CA)	10.41	1.30	1.30
	assign (segid 3A4 and resid 94 and name CA) (segid 3A4 and resid 396 and name CA)	8.19	0.95	0.94
	assign (segid 3A4 and resid 94 and name CA) (segid 3A4 and resid 396 and name CB)	7.95	1.07	1.08
40	assign (segid 3A4 and resid 94 and name CA) (segid 3A4 and resid 397 and name CA)	11.41	0.73	0.73
	assign (segid 3A4 and resid 94 and name CA) (segid 3A4 and resid 397 and name CB)	12.69	0.83	0.83
	assign (segid 3A4 and resid 94 and name CA) (segid 3A4 and resid 398 and name CA)	12.23	0.67	0.68
	assign (segid 3A4 and resid 94 and name CA) (segid 3A4 and resid 398 and name CB)	12.71	0.84	0.84
	assign (segid 3A4 and resid 94 and name CA) (segid 3A4 and resid 399 and name CA)	9.30	0.39	0.38
45	assign (segid 3A4 and resid 94 and name CA) (segid 3A4 and resid 399 and name CB)	7.91	0.45	0.45
	assign (segid 3A4 and resid 94 and name CA) (segid 3A4 and resid 400 and name CA)	9.95	0.29	0.30
	assign (segid 3A4 and resid 94 and name CA) (segid 3A4 and resid 400 and name CB)	10.04	0.36	0.35
	assign (segid 3A4 and resid 94 and name CA) (segid 3A4 and resid 401 and name CA)	13.53	0.23	0.23
	assign (segid 3A4 and resid 94 and name CA) (segid 3A4 and resid 402 and name CA)	13.62	0.34	0.34
50	assign (segid 3A4 and resid 94 and name CA) (segid 3A4 and resid 402 and name CB)	13.19	0.41	0.40
	assign (segid 3A4 and resid 94 and name CA) (segid 3A4 and resid 403 and name CA)	11.94	0.55	0.55
	assign (segid 3A4 and resid 94 and name CA) (segid 3A4 and resid 403 and name CB)	10.53	0.59	0.60
	assign (segid 3A4 and resid 94 and name CA) (segid 3A4 and resid 404 and name CA)	14.19	0.58	0.57
	assign (segid 3A4 and resid 94 and name CA) (segid 3A4 and resid 404 and name CB)	14.33	0.57	0.56
55	assign (segid 3A4 and resid 94 and name CA) (segid 3A4 and resid 405 and name CA)	17.15	0.49	0.49
	assign (segid 3A4 and resid 94 and name CA) (segid 3A4 and resid 405 and name CB)	17.55	0.40	0.39
	assign (segid 3A4 and resid 94 and name CA) (segid 3A4 and resid 406 and name CA)	16.94	0.69	0.70
	assign (segid 3A4 and resid 94 and name CA) (segid 3A4 and resid 407 and name CA)	16.84	0.81	0.80
	assign (segid 3A4 and resid 94 and name CA) (segid 3A4 and resid 407 and name CB)	15.71	0.85	0.85
60	assign (segid 3A4 and resid 94 and name CA) (segid 3A4 and resid 94 and name C)	1.53	0.01	0.01
	assign (segid 3A4 and resid 94 and name CA) (segid 3A4 and resid 94 and name CB)	1.53	0.01	0.01
	assign (segid 3A4 and resid 94 and name CA) (segid 3A4 and resid 94 and name CG)	2.56	0.04	0.05
	assign (segid 3A4 and resid 94 and name CA) (segid 3A4 and resid 94 and name O)	2.38	0.02	0.03
	assign (segid 3A4 and resid 94 and name CA) (segid 3A4 and resid 95 and name C)	4.50	0.09	0.08
65	assign (segid 3A4 and resid 94 and name CA) (segid 3A4 and resid 95 and name CA)	3.82	0.02	0.03
	assign (segid 3A4 and resid 94 and name CA) (segid 3A4 and resid 95 and name CB)	4.88	0.06	0.05
	assign (segid 3A4 and resid 94 and name CA) (segid 3A4 and resid 95 and name N)	2.45	0.02	0.02
	assign (segid 3A4 and resid 94 and name CA) (segid 3A4 and resid 95 and name O)	5.39	0.10	0.11
	assign (segid 3A4 and resid 94 and name CA) (segid 3A4 and resid 96 and name C)	5.68	0.18	0.18
	assign (segid 3A4 and resid 94 and name CA) (segid 3A4 and resid 96 and name CA)	5.64	0.19	0.20
70	assign (segid 3A4 and resid 94 and name CA) (segid 3A4 and resid 96 and name CB)	6.06	0.23	0.23
	assign (segid 3A4 and resid 94 and name CA) (segid 3A4 and resid 96 and name N)	4.55	0.18	0.17
	assign (segid 3A4 and resid 94 and name CA) (segid 3A4 and resid 96 and name O)	6.81	0.17	0.16
	assign (segid 3A4 and resid 94 and name CA) (segid 3A4 and resid 97 and name C)	5.83	0.13	0.14
75	assign (segid 3A4 and resid 94 and name CA) (segid 3A4 and resid 97 and name CA)	5.28	0.18	0.18
	assign (segid 3A4 and resid 94 and name CA) (segid 3A4 and resid 97 and name CB)	4.67	0.26	0.25
	assign (segid 3A4 and resid 94 and name CA) (segid 3A4 and resid 97 and name N)	4.74	0.19	0.19
	assign (segid 3A4 and resid 94 and name CA) (segid 3A4 and resid 97 and name O)	6.96	0.12	0.13
	assign (segid 3A4 and resid 94 and name CA) (segid 3A4 and resid 98 and name CA)	6.32	0.26	0.25
80	assign (segid 3A4 and resid 94 and name CA) (segid 3A4 and resid 98 and name CB)	6.07	0.44	0.44
	assign (segid 3A4 and resid 94 and name CA) (segid 3A4 and resid 98 and name N)	5.34	0.22	0.21
	assign (segid 3A4 and resid 94 and name CA) (segid 3A4 and resid 99 and name CA)	8.94	0.50	0.49
	assign (segid 3A4 and resid 94 and name CA) (segid 3A4 and resid 99 and name CB)	9.04	0.64	0.63

	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 100 and name CA)	10.77	0.25	0.26
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 100 and name CB)	10.43	0.23	0.23
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 101 and name CA)	10.94	0.37	0.37
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 101 and name CB)	10.04	0.51	0.50
5	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 102 and name CA)	12.49	0.29	0.29
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 103 and name CA)	14.90	0.28	0.28
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 103 and name CB)	14.76	0.31	0.32
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 104 and name CA)	15.87	0.30	0.29
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 104 and name CB)	15.15	0.41	0.40
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 105 and name CA)	16.60	0.31	0.31
10	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 105 and name CB)	15.76	0.31	0.30
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 106 and name CA)	18.60	0.29	0.29
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 106 and name CB)	18.23	0.38	0.38
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 126 and name CA)	17.95	0.41	0.40
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 127 and name CA)	17.87	0.78	0.78
15	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 128 and name CA)	15.69	1.29	1.30
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 128 and name CB)	16.20	1.50	1.51
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 129 and name CA)	13.12	0.85	0.86
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 129 and name CB)	13.18	0.66	0.66
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 130 and name CA)	12.62	0.79	0.78
20	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 130 and name CB)	13.66	0.95	0.94
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 131 and name CA)	13.23	0.86	0.86
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 131 and name CB)	14.41	1.12	1.12
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 132 and name CA)	11.12	1.72	1.73
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 132 and name CB)	11.24	1.97	1.98
25	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 133 and name CA)	8.86	0.87	0.87
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 133 and name CB)	8.86	1.05	1.05
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 134 and name CA)	10.38	0.72	0.72
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 135 and name CA)	11.12	1.50	1.49
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 135 and name CB)	11.73	1.98	1.99
30	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 136 and name CA)	8.63	1.85	1.85
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 136 and name CB)	7.75	2.01	2.02
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 137 and name CA)	8.54	0.97	0.97
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 138 and name CA)	11.75	0.67	0.68
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 138 and name CB)	12.68	0.60	0.60
35	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 139 and name CA)	12.42	1.29	1.30
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 140 and name CA)	14.80	1.11	1.11
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 140 and name CB)	15.24	0.78	0.78
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 141 and name CA)	16.14	1.59	1.59
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 205 and name CB)	18.62	0.81	0.82
40	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 219 and name CA)	10.29	1.44	1.45
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 219 and name CB)	10.92	1.47	1.46
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 220 and name CA)	10.92	0.97	0.97
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 220 and name CB)	10.51	0.89	0.88
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 221 and name CA)	14.34	1.00	1.01
45	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 221 and name CB)	14.87	1.01	1.01
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 222 and name CA)	15.31	1.20	1.21
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 222 and name CB)	14.89	1.27	1.27
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 223 and name CA)	14.40	1.05	1.06
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 223 and name CB)	13.15	0.99	1.00
50	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 224 and name CA)	16.39	1.03	1.03
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 224 and name CB)	16.22	1.04	1.04
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 247 and name CA)	18.10	1.10	1.11
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 247 and name CB)	17.66	1.15	1.14
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 248 and name CA)	16.46	0.96	0.96
55	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 248 and name CB)	16.88	0.96	0.96
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 249 and name CA)	18.73	0.79	0.80
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 250 and name CA)	17.91	0.82	0.82
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 250 and name CB)	18.23	0.84	0.84
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 251 and name CA)	14.17	0.76	0.76
60	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 251 and name CB)	13.30	0.83	0.82
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 252 and name CA)	15.10	0.53	0.53
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 252 and name CB)	16.01	0.56	0.57
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 253 and name CA)	17.83	0.57	0.58
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 254 and name CA)	16.50	0.97	0.97
65	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 255 and name CA)	13.63	1.26	1.27
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 256 and name CA)	15.11	0.70	0.71
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 257 and name CA)	18.22	0.74	0.75
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 258 and name CA)	17.42	0.81	0.81
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 258 and name CB)	16.95	0.90	0.90
70	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 259 and name CA)	14.84	0.55	0.56
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 259 and name CB)	13.45	0.54	0.54
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 260 and name CA)	17.17	0.46	0.45
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 260 and name CB)	17.75	0.60	0.60
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 262 and name CA)	18.66	0.66	0.65
75	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 262 and name CB)	17.50	0.78	0.78
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 263 and name CA)	18.02	0.25	0.24
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 263 and name CB)	17.11	0.18	0.18
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 306 and name CA)	17.44	1.07	1.07
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 309 and name CA)	18.20	0.82	0.81
80	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 309 and name CB)	16.74	0.83	0.83
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 384 and name CA)	18.43	1.18	1.19
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 384 and name CB)	17.27	1.16	1.16

	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 391 and name CA)	15.89	1.28	1.28
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 391 and name CB)	15.57	1.27	1.27
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 392 and name CA)	13.31	1.34	1.35
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 392 and name CB)	13.52	1.30	1.30
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 393 and name CA)	10.67	1.23	1.23
5	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 394 and name CA)	11.99	1.33	1.33
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 394 and name CB)	13.12	1.45	1.44
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 395 and name CA)	9.26	1.47	1.46
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 396 and name CA)	6.97	0.93	0.92
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 396 and name CB)	6.67	1.00	0.99
10	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 397 and name CA)	10.24	0.71	0.70
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 397 and name CB)	11.46	0.82	0.82
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 398 and name CA)	11.29	0.75	0.75
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 398 and name CB)	11.77	0.96	0.97
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 399 and name CA)	8.66	0.42	0.41
15	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 399 and name CB)	7.29	0.45	0.45
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 400 and name CA)	9.29	0.39	0.38
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 400 and name CB)	9.24	0.47	0.46
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 401 and name CA)	12.84	0.29	0.29
20	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 402 and name CA)	13.22	0.36	0.35
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 402 and name CB)	12.79	0.43	0.44
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 403 and name CA)	11.83	0.54	0.54
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 403 and name CB)	10.46	0.62	0.63
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 404 and name CA)	13.95	0.58	0.58
25	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 404 and name CB)	13.97	0.56	0.56
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 405 and name CA)	16.88	0.46	0.46
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 405 and name CB)	17.18	0.37	0.37
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 406 and name CA)	16.93	0.62	0.62
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 407 and name CA)	16.99	0.76	0.77
30	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 407 and name CB)	15.90	0.82	0.82
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 94 and name CG)	1.51	0.01	0.01
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 95 and name C)	5.45	0.04	0.05
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 95 and name CA)	4.59	0.05	0.06
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 95 and name CB)	5.62	0.14	0.15
35	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 95 and name N)	3.34	0.08	0.09
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 95 and name O)	6.19	0.11	0.12
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 96 and name C)	6.79	0.09	0.09
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 96 and name CA)	6.88	0.12	0.12
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 96 and name CB)	7.43	0.17	0.17
40	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 96 and name N)	5.75	0.13	0.14
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 97 and name C)	6.38	0.26	0.26
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 97 and name CA)	6.08	0.15	0.14
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 97 and name CB)	5.31	0.13	0.12
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 97 and name N)	5.79	0.10	0.10
45	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 97 and name O)	7.42	0.23	0.22
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 98 and name CA)	6.50	0.50	0.49
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 98 and name CB)	6.08	0.71	0.71
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 98 and name N)	5.75	0.42	0.43
50	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 99 and name CA)	9.54	0.63	0.64
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 99 and name CB)	9.82	0.75	0.75
	assign (segid 3A4 and resid 94 and name CB) (segid 3A4 and resid 99 and name N)	6.86	0.06	0.07
	assign (segid 3A4 and resid 94 and name CG) (segid 3A4 and resid 95 and name C)	6.04	0.07	0.07
	assign (segid 3A4 and resid 94 and name CG) (segid 3A4 and resid 95 and name CB)	7.00	0.17	0.17
	assign (segid 3A4 and resid 94 and name CG) (segid 3A4 and resid 95 and name N)	4.72	0.10	0.11
55	assign (segid 3A4 and resid 94 and name CG) (segid 3A4 and resid 95 and name O)	7.63	0.11	0.11
	assign (segid 3A4 and resid 94 and name CG) (segid 3A4 and resid 96 and name N)	7.03	0.18	0.18
	assign (segid 3A4 and resid 94 and name CG) (segid 3A4 and resid 97 and name CA)	7.02	0.19	0.18
	assign (segid 3A4 and resid 94 and name CG) (segid 3A4 and resid 97 and name CB)	6.00	0.17	0.18
	assign (segid 3A4 and resid 94 and name CG) (segid 3A4 and resid 97 and name N)	6.86	0.16	0.15
60	assign (segid 3A4 and resid 94 and name N) (segid 3A4 and resid 94 and name C)	2.47	0.04	0.04
	assign (segid 3A4 and resid 94 and name N) (segid 3A4 and resid 94 and name CA)	1.45	0.01	0.00
	assign (segid 3A4 and resid 94 and name N) (segid 3A4 and resid 94 and name CB)	2.45	0.03	0.02
	assign (segid 3A4 and resid 94 and name N) (segid 3A4 and resid 94 and name CG)	3.04	0.10	0.11
	assign (segid 3A4 and resid 94 and name N) (segid 3A4 and resid 94 and name O)	3.57	0.05	0.06
65	assign (segid 3A4 and resid 94 and name N) (segid 3A4 and resid 95 and name C)	4.99	0.21	0.20
	assign (segid 3A4 and resid 94 and name N) (segid 3A4 and resid 95 and name CA)	4.19	0.05	0.06
	assign (segid 3A4 and resid 94 and name N) (segid 3A4 and resid 95 and name CB)	4.87	0.05	0.06
	assign (segid 3A4 and resid 94 and name N) (segid 3A4 and resid 95 and name N)	2.76	0.05	0.06
	assign (segid 3A4 and resid 94 and name N) (segid 3A4 and resid 95 and name O)	6.05	0.18	0.19
70	assign (segid 3A4 and resid 94 and name N) (segid 3A4 and resid 96 and name C)	6.34	0.43	0.43
	assign (segid 3A4 and resid 94 and name N) (segid 3A4 and resid 96 and name CA)	6.01	0.45	0.45
	assign (segid 3A4 and resid 94 and name N) (segid 3A4 and resid 96 and name CB)	6.18	0.54	0.54
	assign (segid 3A4 and resid 94 and name N) (segid 3A4 and resid 96 and name N)	4.85	0.37	0.37
	assign (segid 3A4 and resid 94 and name N) (segid 3A4 and resid 97 and name C)	7.01	0.24	0.24
75	assign (segid 3A4 and resid 94 and name N) (segid 3A4 and resid 97 and name CA)	6.32	0.37	0.38
	assign (segid 3A4 and resid 94 and name N) (segid 3A4 and resid 97 and name CB)	5.80	0.41	0.42
	assign (segid 3A4 and resid 94 and name N) (segid 3A4 and resid 97 and name N)	5.58	0.41	0.41
	assign (segid 3A4 and resid 94 and name N) (segid 3A4 and resid 98 and name CA)	7.52	0.18	0.18
	assign (segid 3A4 and resid 94 and name N) (segid 3A4 and resid 98 and name N)	6.52	0.17	0.18
80	assign (segid 3A4 and resid 94 and name O) (segid 3A4 and resid 100 and name CB)	7.71	0.17	0.17
	assign (segid 3A4 and resid 94 and name O) (segid 3A4 and resid 100 and name N)	6.93	0.27	0.28
	assign (segid 3A4 and resid 94 and name O) (segid 3A4 and resid 94 and name CB)	3.06	0.14	0.13
	assign (segid 3A4 and resid 94 and name O) (segid 3A4 and resid 94 and name CG)	4.39	0.12	0.13

	assign	(segid 3A4 and resid 94 and name O)	(segid 3A4 and resid 95 and name C)	2.92	0.04	0.04
	assign	(segid 3A4 and resid 94 and name O)	(segid 3A4 and resid 95 and name CA)	2.77	0.03	0.02
	assign	(segid 3A4 and resid 94 and name O)	(segid 3A4 and resid 95 and name CB)	4.24	0.06	0.06
	assign	(segid 3A4 and resid 94 and name O)	(segid 3A4 and resid 95 and name N)	2.22	0.02	0.02
5	assign	(segid 3A4 and resid 94 and name O)	(segid 3A4 and resid 95 and name O)	3.44	0.11	0.11
	assign	(segid 3A4 and resid 94 and name O)	(segid 3A4 and resid 96 and name C)	3.97	0.07	0.06
	assign	(segid 3A4 and resid 94 and name O)	(segid 3A4 and resid 96 and name CA)	4.26	0.07	0.07
	assign	(segid 3A4 and resid 94 and name O)	(segid 3A4 and resid 96 and name CB)	5.17	0.05	0.06
	assign	(segid 3A4 and resid 94 and name O)	(segid 3A4 and resid 96 and name N)	3.34	0.06	0.05
10	assign	(segid 3A4 and resid 94 and name O)	(segid 3A4 and resid 96 and name O)	4.96	0.10	0.09
	assign	(segid 3A4 and resid 94 and name O)	(segid 3A4 and resid 97 and name C)	3.71	0.10	0.10
	assign	(segid 3A4 and resid 94 and name O)	(segid 3A4 and resid 97 and name CA)	3.53	0.08	0.08
	assign	(segid 3A4 and resid 94 and name O)	(segid 3A4 and resid 97 and name CB)	3.40	0.16	0.17
	assign	(segid 3A4 and resid 94 and name O)	(segid 3A4 and resid 97 and name N)	3.06	0.06	0.07
15	assign	(segid 3A4 and resid 94 and name O)	(segid 3A4 and resid 97 and name O)	4.87	0.07	0.08
	assign	(segid 3A4 and resid 94 and name O)	(segid 3A4 and resid 98 and name C)	5.20	0.30	0.30
	assign	(segid 3A4 and resid 94 and name O)	(segid 3A4 and resid 98 and name CA)	4.04	0.22	0.21
	assign	(segid 3A4 and resid 94 and name O)	(segid 3A4 and resid 98 and name CB)	3.96	0.33	0.33
	assign	(segid 3A4 and resid 94 and name O)	(segid 3A4 and resid 98 and name N)	3.04	0.21	0.20
20	assign	(segid 3A4 and resid 94 and name O)	(segid 3A4 and resid 98 and name O)	6.27	0.20	0.20
	assign	(segid 3A4 and resid 94 and name O)	(segid 3A4 and resid 99 and name CA)	6.64	0.49	0.49
	assign	(segid 3A4 and resid 94 and name O)	(segid 3A4 and resid 99 and name N)	5.27	0.47	0.48
	assign	(segid 3A4 and resid 95 and name C)	(segid 3A4 and resid 100 and name N)	6.22	0.55	0.55
25	assign	(segid 3A4 and resid 95 and name C)	(segid 3A4 and resid 95 and name CB)	2.48	0.04	0.04
	assign	(segid 3A4 and resid 95 and name C)	(segid 3A4 and resid 95 and name O)	1.24	0.01	0.01
	assign	(segid 3A4 and resid 95 and name C)	(segid 3A4 and resid 96 and name C)	3.01	0.05	0.06
	assign	(segid 3A4 and resid 95 and name C)	(segid 3A4 and resid 96 and name CA)	2.44	0.02	0.02
	assign	(segid 3A4 and resid 95 and name C)	(segid 3A4 and resid 96 and name CB)	3.69	0.03	0.03
	assign	(segid 3A4 and resid 95 and name C)	(segid 3A4 and resid 96 and name N)	1.33	0.01	0.01
30	assign	(segid 3A4 and resid 95 and name C)	(segid 3A4 and resid 96 and name O)	3.91	0.12	0.13
	assign	(segid 3A4 and resid 95 and name C)	(segid 3A4 and resid 97 and name C)	4.47	0.06	0.06
	assign	(segid 3A4 and resid 95 and name C)	(segid 3A4 and resid 97 and name CA)	4.37	0.08	0.07
	assign	(segid 3A4 and resid 95 and name C)	(segid 3A4 and resid 97 and name CB)	5.15	0.14	0.14
	assign	(segid 3A4 and resid 95 and name C)	(segid 3A4 and resid 97 and name N)	3.20	0.11	0.11
35	assign	(segid 3A4 and resid 95 and name C)	(segid 3A4 and resid 97 and name O)	5.57	0.10	0.09
	assign	(segid 3A4 and resid 95 and name C)	(segid 3A4 and resid 98 and name C)	4.98	0.34	0.34
	assign	(segid 3A4 and resid 95 and name C)	(segid 3A4 and resid 98 and name CA)	4.54	0.10	0.10
	assign	(segid 3A4 and resid 95 and name C)	(segid 3A4 and resid 98 and name CB)	4.36	0.12	0.12
	assign	(segid 3A4 and resid 95 and name C)	(segid 3A4 and resid 98 and name N)	3.76	0.10	0.09
40	assign	(segid 3A4 and resid 95 and name C)	(segid 3A4 and resid 98 and name O)	6.17	0.32	0.33
	assign	(segid 3A4 and resid 95 and name C)	(segid 3A4 and resid 99 and name CA)	5.35	0.72	0.73
	assign	(segid 3A4 and resid 95 and name C)	(segid 3A4 and resid 99 and name CB)	5.00	0.90	0.90
	assign	(segid 3A4 and resid 95 and name C)	(segid 3A4 and resid 99 and name N)	4.36	0.57	0.58
45	assign	(segid 3A4 and resid 95 and name CA)	(segid 3A4 and resid 100 and name CA)	8.78	0.39	0.39
	assign	(segid 3A4 and resid 95 and name CA)	(segid 3A4 and resid 100 and name CB)	8.83	0.30	0.30
	assign	(segid 3A4 and resid 95 and name CA)	(segid 3A4 and resid 101 and name CA)	10.01	0.18	0.18
	assign	(segid 3A4 and resid 95 and name CA)	(segid 3A4 and resid 101 and name CB)	9.61	0.38	0.39
	assign	(segid 3A4 and resid 95 and name CA)	(segid 3A4 and resid 102 and name CA)	10.59	0.32	0.33
50	assign	(segid 3A4 and resid 95 and name CA)	(segid 3A4 and resid 103 and name CA)	12.48	0.46	0.46
	assign	(segid 3A4 and resid 95 and name CA)	(segid 3A4 and resid 103 and name CB)	12.14	0.53	0.53
	assign	(segid 3A4 and resid 95 and name CA)	(segid 3A4 and resid 104 and name CA)	14.39	0.20	0.21
	assign	(segid 3A4 and resid 95 and name CA)	(segid 3A4 and resid 104 and name CB)	14.04	0.17	0.18
	assign	(segid 3A4 and resid 95 and name CA)	(segid 3A4 and resid 105 and name CA)	15.38	0.21	0.22
55	assign	(segid 3A4 and resid 95 and name CA)	(segid 3A4 and resid 105 and name CB)	14.65	0.24	0.25
	assign	(segid 3A4 and resid 95 and name CA)	(segid 3A4 and resid 106 and name CA)	16.57	0.45	0.44
	assign	(segid 3A4 and resid 95 and name CA)	(segid 3A4 and resid 106 and name CB)	15.88	0.56	0.55
	assign	(segid 3A4 and resid 95 and name CA)	(segid 3A4 and resid 107 and name CA)	18.44	0.43	0.43
	assign	(segid 3A4 and resid 95 and name CA)	(segid 3A4 and resid 107 and name CB)	18.02	0.41	0.42
	assign	(segid 3A4 and resid 95 and name CA)	(segid 3A4 and resid 108 and name CB)	19.56	0.13	0.13
60	assign	(segid 3A4 and resid 95 and name CA)	(segid 3A4 and resid 128 and name CA)	16.44	1.74	1.74
	assign	(segid 3A4 and resid 95 and name CA)	(segid 3A4 and resid 129 and name CA)	13.93	0.98	0.98
	assign	(segid 3A4 and resid 95 and name CA)	(segid 3A4 and resid 129 and name CB)	14.05	0.91	0.91
	assign	(segid 3A4 and resid 95 and name CA)	(segid 3A4 and resid 130 and name CA)	14.30	0.93	0.92
65	assign	(segid 3A4 and resid 95 and name CA)	(segid 3A4 and resid 130 and name CB)	15.33	1.07	1.08
	assign	(segid 3A4 and resid 95 and name CA)	(segid 3A4 and resid 131 and name CA)	15.16	1.14	1.14
	assign	(segid 3A4 and resid 95 and name CA)	(segid 3A4 and resid 131 and name CB)	16.13	1.59	1.59
	assign	(segid 3A4 and resid 95 and name CA)	(segid 3A4 and resid 132 and name CA)	12.90	1.81	1.81
	assign	(segid 3A4 and resid 95 and name CA)	(segid 3A4 and resid 132 and name CB)	12.65	2.02	2.02
	assign	(segid 3A4 and resid 95 and name CA)	(segid 3A4 and resid 133 and name CA)	11.34	0.69	0.69
70	assign	(segid 3A4 and resid 95 and name CA)	(segid 3A4 and resid 133 and name CB)	11.20	1.24	1.24
	assign	(segid 3A4 and resid 95 and name CA)	(segid 3A4 and resid 134 and name CA)	13.44	0.41	0.41
	assign	(segid 3A4 and resid 95 and name CA)	(segid 3A4 and resid 135 and name CA)	13.97	1.71	1.71
	assign	(segid 3A4 and resid 95 and name CA)	(segid 3A4 and resid 135 and name CB)	14.22	2.37	2.37
	assign	(segid 3A4 and resid 95 and name CA)	(segid 3A4 and resid 136 and name CA)	11.77	1.45	1.45
75	assign	(segid 3A4 and resid 95 and name CA)	(segid 3A4 and resid 136 and name CB)	10.75	1.39	1.40
	assign	(segid 3A4 and resid 95 and name CA)	(segid 3A4 and resid 137 and name CA)	12.35	0.74	0.74
	assign	(segid 3A4 and resid 95 and name CA)	(segid 3A4 and resid 138 and name CA)	15.48	0.46	0.47
	assign	(segid 3A4 and resid 95 and name CA)	(segid 3A4 and resid 138 and name CB)	16.39	0.11	0.11
	assign	(segid 3A4 and resid 95 and name CA)	(segid 3A4 and resid 139 and name CA)	15.58	1.39	1.39
80	assign	(segid 3A4 and resid 95 and name CA)	(segid 3A4 and resid 140 and name CA)	17.65	1.38	1.38
	assign	(segid 3A4 and resid 95 and name CA)	(segid 3A4 and resid 140 and name CB)	18.18	0.94	0.94
	assign	(segid 3A4 and resid 95 and name CA)	(segid 3A4 and resid 219 and name CA)	13.98	1.38	1.38
	assign	(segid 3A4 and resid 95 and name CA)	(segid 3A4 and resid 219 and name CB)	14.54	1.42	1.43

	assign (segid 3A4 and resid 95 and name CA) (segid 3A4 and resid 220 and name CA)	15.09	1.14	1.15
	assign (segid 3A4 and resid 95 and name CA) (segid 3A4 and resid 220 and name CB)	14.76	1.11	1.11
	assign (segid 3A4 and resid 95 and name CA) (segid 3A4 and resid 223 and name CB)	17.08	1.25	1.25
	assign (segid 3A4 and resid 95 and name CA) (segid 3A4 and resid 251 and name CA)	18.10	0.72	0.72
5	assign (segid 3A4 and resid 95 and name CA) (segid 3A4 and resid 251 and name CB)	17.35	0.82	0.82
	assign (segid 3A4 and resid 95 and name CA) (segid 3A4 and resid 252 and name CA)	18.66	0.61	0.61
	assign (segid 3A4 and resid 95 and name CA) (segid 3A4 and resid 255 and name CA)	16.64	0.98	0.97
	assign (segid 3A4 and resid 95 and name CA) (segid 3A4 and resid 256 and name CA)	17.63	0.59	0.60
	assign (segid 3A4 and resid 95 and name CA) (segid 3A4 and resid 259 and name CA)	16.25	0.43	0.42
10	assign (segid 3A4 and resid 95 and name CA) (segid 3A4 and resid 259 and name CB)	14.95	0.49	0.49
	assign (segid 3A4 and resid 95 and name CA) (segid 3A4 and resid 260 and name CA)	18.25	0.63	0.63
	assign (segid 3A4 and resid 95 and name CA) (segid 3A4 and resid 262 and name CA)	19.22	0.28	0.28
	assign (segid 3A4 and resid 95 and name CA) (segid 3A4 and resid 262 and name CB)	18.14	0.33	0.33
	assign (segid 3A4 and resid 95 and name CA) (segid 3A4 and resid 263 and name CA)	17.92	0.49	0.49
15	assign (segid 3A4 and resid 95 and name CA) (segid 3A4 and resid 263 and name CB)	17.03	0.58	0.58
	assign (segid 3A4 and resid 95 and name CA) (segid 3A4 and resid 303 and name CA)	17.80	1.15	1.15
	assign (segid 3A4 and resid 95 and name CA) (segid 3A4 and resid 305 and name CA)	16.71	1.03	1.04
	assign (segid 3A4 and resid 95 and name CA) (segid 3A4 and resid 305 and name CB)	15.59	1.13	1.13
20	assign (segid 3A4 and resid 95 and name CA) (segid 3A4 and resid 306 and name CA)	15.65	0.84	0.84
	assign (segid 3A4 and resid 95 and name CA) (segid 3A4 and resid 309 and name CA)	17.28	0.67	0.67
	assign (segid 3A4 and resid 95 and name CA) (segid 3A4 and resid 309 and name CB)	15.78	0.68	0.68
	assign (segid 3A4 and resid 95 and name CA) (segid 3A4 and resid 391 and name CB)	18.19	0.82	0.81
	assign (segid 3A4 and resid 95 and name CA) (segid 3A4 and resid 392 and name CA)	16.59	1.00	1.00
	assign (segid 3A4 and resid 95 and name CA) (segid 3A4 and resid 392 and name CB)	17.06	1.01	1.02
25	assign (segid 3A4 and resid 95 and name CA) (segid 3A4 and resid 393 and name CA)	13.76	0.83	0.82
	assign (segid 3A4 and resid 95 and name CA) (segid 3A4 and resid 394 and name CA)	14.04	0.85	0.85
	assign (segid 3A4 and resid 95 and name CA) (segid 3A4 and resid 394 and name CB)	15.06	0.95	0.96
	assign (segid 3A4 and resid 95 and name CA) (segid 3A4 and resid 395 and name CA)	10.80	1.00	1.00
	assign (segid 3A4 and resid 95 and name CA) (segid 3A4 and resid 396 and name CA)	9.02	0.66	0.65
30	assign (segid 3A4 and resid 95 and name CA) (segid 3A4 and resid 396 and name CB)	9.37	0.81	0.81
	assign (segid 3A4 and resid 95 and name CA) (segid 3A4 and resid 397 and name CA)	11.65	0.43	0.43
	assign (segid 3A4 and resid 95 and name CA) (segid 3A4 and resid 397 and name CB)	13.06	0.45	0.45
	assign (segid 3A4 and resid 95 and name CA) (segid 3A4 and resid 398 and name CA)	11.42	0.39	0.39
	assign (segid 3A4 and resid 95 and name CA) (segid 3A4 and resid 398 and name CB)	11.86	0.56	0.56
35	assign (segid 3A4 and resid 95 and name CA) (segid 3A4 and resid 399 and name CA)	7.93	0.40	0.40
	assign (segid 3A4 and resid 95 and name CA) (segid 3A4 and resid 399 and name CB)	6.77	0.46	0.45
	assign (segid 3A4 and resid 95 and name CA) (segid 3A4 and resid 400 and name CA)	8.95	0.77	0.77
	assign (segid 3A4 and resid 95 and name CA) (segid 3A4 and resid 400 and name CB)	9.58	0.75	0.74
	assign (segid 3A4 and resid 95 and name CA) (segid 3A4 and resid 401 and name CA)	12.14	0.68	0.69
40	assign (segid 3A4 and resid 95 and name CA) (segid 3A4 and resid 401 and name CB)	11.36	0.74	0.74
	assign (segid 3A4 and resid 95 and name CA) (segid 3A4 and resid 402 and name CA)	10.85	0.65	0.66
	assign (segid 3A4 and resid 95 and name CA) (segid 3A4 and resid 402 and name CB)	9.33	1.12	1.12
	assign (segid 3A4 and resid 95 and name CA) (segid 3A4 and resid 403 and name CA)	8.01	1.18	1.18
	assign (segid 3A4 and resid 95 and name CA) (segid 3A4 and resid 403 and name CB)	12.12	1.18	1.18
45	assign (segid 3A4 and resid 95 and name CA) (segid 3A4 and resid 404 and name CA)	12.61	1.10	1.10
	assign (segid 3A4 and resid 95 and name CA) (segid 3A4 and resid 405 and name CA)	14.82	1.13	1.13
	assign (segid 3A4 and resid 95 and name CA) (segid 3A4 and resid 405 and name CB)	15.28	1.02	1.01
	assign (segid 3A4 and resid 95 and name CA) (segid 3A4 and resid 406 and name CA)	14.01	1.28	1.29
	assign (segid 3A4 and resid 95 and name CA) (segid 3A4 and resid 407 and name CA)	14.01	1.42	1.43
50	assign (segid 3A4 and resid 95 and name CA) (segid 3A4 and resid 407 and name CB)	13.00	1.48	1.47
	assign (segid 3A4 and resid 95 and name CA) (segid 3A4 and resid 95 and name C)	1.52	0.00	0.00
	assign (segid 3A4 and resid 95 and name CA) (segid 3A4 and resid 95 and name CB)	1.52	0.03	0.03
	assign (segid 3A4 and resid 95 and name CA) (segid 3A4 and resid 95 and name O)	2.40	0.02	0.01
	assign (segid 3A4 and resid 95 and name CA) (segid 3A4 and resid 96 and name C)	4.40	0.05	0.05
55	assign (segid 3A4 and resid 95 and name CA) (segid 3A4 and resid 96 and name CA)	3.82	0.03	0.02
	assign (segid 3A4 and resid 95 and name CA) (segid 3A4 and resid 96 and name CB)	4.84	0.03	0.03
	assign (segid 3A4 and resid 95 and name CA) (segid 3A4 and resid 96 and name N)	2.44	0.03	0.02
	assign (segid 3A4 and resid 95 and name CA) (segid 3A4 and resid 96 and name O)	5.37	0.12	0.12
	assign (segid 3A4 and resid 95 and name CA) (segid 3A4 and resid 97 and name C)	5.39	0.09	0.08
60	assign (segid 3A4 and resid 95 and name CA) (segid 3A4 and resid 97 and name CA)	5.34	0.10	0.09
	assign (segid 3A4 and resid 95 and name CA) (segid 3A4 and resid 97 and name CB)	5.78	0.18	0.19
	assign (segid 3A4 and resid 95 and name CA) (segid 3A4 and resid 97 and name N)	4.29	0.11	0.12
	assign (segid 3A4 and resid 95 and name CA) (segid 3A4 and resid 97 and name O)	6.52	0.10	0.10
	assign (segid 3A4 and resid 95 and name CA) (segid 3A4 and resid 98 and name C)	5.79	0.36	0.35
65	assign (segid 3A4 and resid 95 and name CA) (segid 3A4 and resid 98 and name CA)	5.09	0.11	0.11
	assign (segid 3A4 and resid 95 and name CA) (segid 3A4 and resid 98 and name CB)	4.52	0.15	0.14
	assign (segid 3A4 and resid 95 and name CA) (segid 3A4 and resid 98 and name N)	4.47	0.08	0.09
	assign (segid 3A4 and resid 95 and name CA) (segid 3A4 and resid 98 and name O)	6.94	0.31	0.32
	assign (segid 3A4 and resid 95 and name CA) (segid 3A4 and resid 99 and name CA)	6.48	0.72	0.72
70	assign (segid 3A4 and resid 95 and name CA) (segid 3A4 and resid 99 and name CB)	6.23	0.91	0.91
	assign (segid 3A4 and resid 95 and name CA) (segid 3A4 and resid 99 and name N)	5.39	0.59	0.60
	assign (segid 3A4 and resid 95 and name CB) (segid 3A4 and resid 100 and name CA)	9.82	0.49	0.48
	assign (segid 3A4 and resid 95 and name CB) (segid 3A4 and resid 100 and name CB)	9.94	0.38	0.39
	assign (segid 3A4 and resid 95 and name CB) (segid 3A4 and resid 101 and name CA)	11.25	0.16	0.16
75	assign (segid 3A4 and resid 95 and name CB) (segid 3A4 and resid 101 and name CB)	10.93	0.36	0.36
	assign (segid 3A4 and resid 95 and name CB) (segid 3A4 and resid 102 and name CA)	11.51	0.39	0.40
	assign (segid 3A4 and resid 95 and name CB) (segid 3A4 and resid 103 and name CA)	13.27	0.61	0.60
	assign (segid 3A4 and resid 95 and name CB) (segid 3A4 and resid 103 and name CB)	12.88	0.69	0.68
	assign (segid 3A4 and resid 95 and name CB) (segid 3A4 and resid 104 and name CA)	15.44	0.31	0.32
80	assign (segid 3A4 and resid 95 and name CB) (segid 3A4 and resid 104 and name CB)	15.19	0.23	0.24
	assign (segid 3A4 and resid 95 and name CB) (segid 3A4 and resid 105 and name CA)	16.42	0.26	0.25
	assign (segid 3A4 and resid 95 and name CB) (segid 3A4 and resid 105 and name CB)	15.69	0.28	0.27
	assign (segid 3A4 and resid 95 and name CB) (segid 3A4 and resid 106 and name CA)	17.34	0.57	0.58

	assign (segid 3A4 and resid 95 and name CB) (segid 3A4 and resid 106 and name CB)	16.55	0.71	0.72
	assign (segid 3A4 and resid 95 and name CB) (segid 3A4 and resid 129 and name CA)	15.19	1.05	1.05
	assign (segid 3A4 and resid 95 and name CB) (segid 3A4 and resid 129 and name CB)	15.23	1.02	1.03
	assign (segid 3A4 and resid 95 and name CB) (segid 3A4 and resid 130 and name CA)	15.58	1.05	1.06
	assign (segid 3A4 and resid 95 and name CB) (segid 3A4 and resid 130 and name CB)	16.57	1.24	1.24
5	assign (segid 3A4 and resid 95 and name CB) (segid 3A4 and resid 131 and name CA)	16.55	1.11	1.12
	assign (segid 3A4 and resid 95 and name CB) (segid 3A4 and resid 132 and name CA)	14.36	1.80	1.80
	assign (segid 3A4 and resid 95 and name CB) (segid 3A4 and resid 132 and name CB)	14.09	2.03	2.03
	assign (segid 3A4 and resid 95 and name CB) (segid 3A4 and resid 133 and name CA)	12.78	0.74	0.73
	assign (segid 3A4 and resid 95 and name CB) (segid 3A4 and resid 133 and name CB)	12.58	1.29	1.30
10	assign (segid 3A4 and resid 95 and name CB) (segid 3A4 and resid 134 and name CA)	14.83	0.49	0.49
	assign (segid 3A4 and resid 95 and name CB) (segid 3A4 and resid 135 and name CA)	15.41	1.69	1.68
	assign (segid 3A4 and resid 95 and name CB) (segid 3A4 and resid 135 and name CB)	15.68	2.35	2.35
	assign (segid 3A4 and resid 95 and name CB) (segid 3A4 and resid 136 and name CA)	13.19	1.47	1.47
	assign (segid 3A4 and resid 95 and name CB) (segid 3A4 and resid 136 and name CB)	12.18	1.42	1.42
15	assign (segid 3A4 and resid 95 and name CB) (segid 3A4 and resid 137 and name CA)	13.65	0.79	0.79
	assign (segid 3A4 and resid 95 and name CB) (segid 3A4 and resid 138 and name CA)	16.77	0.50	0.50
	assign (segid 3A4 and resid 95 and name CB) (segid 3A4 and resid 138 and name CB)	17.70	0.46	0.45
	assign (segid 3A4 and resid 95 and name CB) (segid 3A4 and resid 139 and name CA)	16.90	1.40	1.40
20	assign (segid 3A4 and resid 95 and name CB) (segid 3A4 and resid 219 and name CA)	15.03	1.41	1.41
	assign (segid 3A4 and resid 95 and name CB) (segid 3A4 and resid 219 and name CB)	15.68	1.45	1.45
	assign (segid 3A4 and resid 95 and name CB) (segid 3A4 and resid 220 and name CA)	16.08	1.18	1.18
	assign (segid 3A4 and resid 95 and name CB) (segid 3A4 and resid 220 and name CB)	15.78	1.12	1.13
	assign (segid 3A4 and resid 95 and name CB) (segid 3A4 and resid 251 and name CB)	18.42	0.73	0.73
25	assign (segid 3A4 and resid 95 and name CB) (segid 3A4 and resid 255 and name CA)	17.69	0.88	0.88
	assign (segid 3A4 and resid 95 and name CB) (segid 3A4 and resid 256 and name CA)	18.80	0.49	0.50
	assign (segid 3A4 and resid 95 and name CB) (segid 3A4 and resid 259 and name CA)	17.11	0.45	0.46
	assign (segid 3A4 and resid 95 and name CB) (segid 3A4 and resid 259 and name CB)	15.87	0.53	0.53
	assign (segid 3A4 and resid 95 and name CB) (segid 3A4 and resid 262 and name CB)	18.74	0.29	0.30
30	assign (segid 3A4 and resid 95 and name CB) (segid 3A4 and resid 263 and name CB)	17.78	0.71	0.72
	assign (segid 3A4 and resid 95 and name CB) (segid 3A4 and resid 303 and name CA)	17.03	1.24	1.24
	assign (segid 3A4 and resid 95 and name CB) (segid 3A4 and resid 305 and name CA)	16.33	1.21	1.21
	assign (segid 3A4 and resid 95 and name CB) (segid 3A4 and resid 305 and name CB)	15.22	1.29	1.30
	assign (segid 3A4 and resid 95 and name CB) (segid 3A4 and resid 306 and name CA)	15.20	0.96	0.95
35	assign (segid 3A4 and resid 95 and name CB) (segid 3A4 and resid 309 and name CA)	17.23	0.86	0.87
	assign (segid 3A4 and resid 95 and name CB) (segid 3A4 and resid 309 and name CB)	15.73	0.87	0.87
	assign (segid 3A4 and resid 95 and name CB) (segid 3A4 and resid 391 and name CB)	18.57	0.79	0.80
	assign (segid 3A4 and resid 95 and name CB) (segid 3A4 and resid 392 and name CA)	16.99	1.01	1.01
	assign (segid 3A4 and resid 95 and name CB) (segid 3A4 and resid 392 and name CB)	17.54	1.04	1.04
40	assign (segid 3A4 and resid 95 and name CB) (segid 3A4 and resid 393 and name CA)	14.32	0.77	0.78
	assign (segid 3A4 and resid 95 and name CB) (segid 3A4 and resid 394 and name CA)	14.31	0.81	0.82
	assign (segid 3A4 and resid 95 and name CB) (segid 3A4 and resid 394 and name CB)	15.22	0.93	0.93
	assign (segid 3A4 and resid 95 and name CB) (segid 3A4 and resid 395 and name CA)	10.89	0.92	0.93
	assign (segid 3A4 and resid 95 and name CB) (segid 3A4 and resid 396 and name CA)	9.59	0.58	0.58
45	assign (segid 3A4 and resid 95 and name CB) (segid 3A4 and resid 396 and name CB)	10.11	0.73	0.72
	assign (segid 3A4 and resid 95 and name CB) (segid 3A4 and resid 397 and name CA)	12.22	0.43	0.44
	assign (segid 3A4 and resid 95 and name CB) (segid 3A4 and resid 397 and name CB)	13.61	0.43	0.43
	assign (segid 3A4 and resid 95 and name CB) (segid 3A4 and resid 398 and name CA)	11.58	0.46	0.45
	assign (segid 3A4 and resid 95 and name CB) (segid 3A4 and resid 398 and name CB)	11.86	0.56	0.56
50	assign (segid 3A4 and resid 95 and name CB) (segid 3A4 and resid 399 and name CA)	8.11	0.58	0.58
	assign (segid 3A4 and resid 95 and name CB) (segid 3A4 and resid 399 and name CB)	6.99	0.58	0.58
	assign (segid 3A4 and resid 95 and name CB) (segid 3A4 and resid 400 and name CA)	9.64	0.93	0.92
	assign (segid 3A4 and resid 95 and name CB) (segid 3A4 and resid 400 and name CB)	10.42	0.87	0.86
	assign (segid 3A4 and resid 95 and name CB) (segid 3A4 and resid 401 and name CA)	12.56	0.87	0.88
55	assign (segid 3A4 and resid 95 and name CB) (segid 3A4 and resid 402 and name CA)	11.37	0.99	1.00
	assign (segid 3A4 and resid 95 and name CB) (segid 3A4 and resid 402 and name CB)	10.71	0.91	0.91
	assign (segid 3A4 and resid 95 and name CB) (segid 3A4 and resid 403 and name CA)	9.55	1.37	1.36
	assign (segid 3A4 and resid 95 and name CB) (segid 3A4 and resid 403 and name CB)	8.36	1.41	1.40
	assign (segid 3A4 and resid 95 and name CB) (segid 3A4 and resid 404 and name CA)	12.64	1.36	1.36
60	assign (segid 3A4 and resid 95 and name CB) (segid 3A4 and resid 404 and name CB)	13.24	1.25	1.25
	assign (segid 3A4 and resid 95 and name CB) (segid 3A4 and resid 405 and name CA)	15.06	1.37	1.36
	assign (segid 3A4 and resid 95 and name CB) (segid 3A4 and resid 405 and name CB)	15.46	1.25	1.24
	assign (segid 3A4 and resid 95 and name CB) (segid 3A4 and resid 406 and name CA)	13.97	1.56	1.55
	assign (segid 3A4 and resid 95 and name CB) (segid 3A4 and resid 407 and name CA)	14.23	1.67	1.66
	assign (segid 3A4 and resid 95 and name CB) (segid 3A4 and resid 407 and name CB)	13.32	1.71	1.70
65	assign (segid 3A4 and resid 95 and name CB) (segid 3A4 and resid 96 and name C)	5.41	0.07	0.06
	assign (segid 3A4 and resid 95 and name CB) (segid 3A4 and resid 96 and name CA)	4.48	0.06	0.05
	assign (segid 3A4 and resid 95 and name CB) (segid 3A4 and resid 96 and name CB)	5.32	0.04	0.05
	assign (segid 3A4 and resid 95 and name CB) (segid 3A4 and resid 96 and name N)	3.14	0.05	0.05
	assign (segid 3A4 and resid 95 and name CB) (segid 3A4 and resid 96 and name O)	6.32	0.13	0.13
70	assign (segid 3A4 and resid 95 and name CB) (segid 3A4 and resid 97 and name C)	6.78	0.08	0.07
	assign (segid 3A4 and resid 95 and name CB) (segid 3A4 and resid 97 and name CA)	6.70	0.10	0.10
	assign (segid 3A4 and resid 95 and name CB) (segid 3A4 and resid 97 and name CB)	7.22	0.19	0.20
	assign (segid 3A4 and resid 95 and name CB) (segid 3A4 and resid 97 and name N)	5.54	0.11	0.11
	assign (segid 3A4 and resid 95 and name CB) (segid 3A4 and resid 98 and name C)	6.89	0.36	0.36
75	assign (segid 3A4 and resid 95 and name CB) (segid 3A4 and resid 98 and name CA)	6.37	0.08	0.07
	assign (segid 3A4 and resid 95 and name CB) (segid 3A4 and resid 98 and name CB)	5.65	0.11	0.12
	assign (segid 3A4 and resid 95 and name CB) (segid 3A4 and resid 98 and name N)	5.86	0.06	0.07
	assign (segid 3A4 and resid 95 and name CB) (segid 3A4 and resid 99 and name CA)	7.23	0.80	0.80
	assign (segid 3A4 and resid 95 and name CB) (segid 3A4 and resid 99 and name CB)	6.73	1.01	1.02
80	assign (segid 3A4 and resid 95 and name CB) (segid 3A4 and resid 99 and name N)	6.35	0.61	0.60
	assign (segid 3A4 and resid 95 and name CB) (segid 3A4 and resid 399 and name CB)	7.06	0.37	0.38
	assign (segid 3A4 and resid 95 and name N) (segid 3A4 and resid 95 and name C)	2.50	0.06	0.05

	assign (segid 3A4 and resid 95 and name N) (segid 3A4 and resid 95 and name CA)	1.46	0.02	0.01
	assign (segid 3A4 and resid 95 and name N) (segid 3A4 and resid 95 and name CB)	2.45	0.06	0.06
	assign (segid 3A4 and resid 95 and name N) (segid 3A4 and resid 95 and name O)	3.52	0.05	0.05
	assign (segid 3A4 and resid 95 and name N) (segid 3A4 and resid 96 and name C)	4.77	0.10	0.10
	assign (segid 3A4 and resid 95 and name N) (segid 3A4 and resid 96 and name CA)	4.30	0.12	0.12
5	assign (segid 3A4 and resid 95 and name N) (segid 3A4 and resid 96 and name CB)	5.03	0.12	0.13
	assign (segid 3A4 and resid 95 and name N) (segid 3A4 and resid 96 and name N)	2.90	0.12	0.11
	assign (segid 3A4 and resid 95 and name N) (segid 3A4 and resid 96 and name O)	5.88	0.09	0.09
	assign (segid 3A4 and resid 95 and name N) (segid 3A4 and resid 97 and name C)	5.59	0.10	0.10
	assign (segid 3A4 and resid 95 and name N) (segid 3A4 and resid 97 and name CA)	5.29	0.12	0.12
10	assign (segid 3A4 and resid 95 and name N) (segid 3A4 and resid 97 and name CB)	5.37	0.19	0.20
	assign (segid 3A4 and resid 95 and name N) (segid 3A4 and resid 97 and name N)	4.33	0.14	0.14
	assign (segid 3A4 and resid 95 and name N) (segid 3A4 and resid 97 and name O)	6.79	0.10	0.09
	assign (segid 3A4 and resid 95 and name N) (segid 3A4 and resid 98 and name C)	6.56	0.35	0.35
	assign (segid 3A4 and resid 95 and name N) (segid 3A4 and resid 98 and name CA)	5.62	0.18	0.18
15	assign (segid 3A4 and resid 95 and name N) (segid 3A4 and resid 98 and name CB)	5.14	0.28	0.27
	assign (segid 3A4 and resid 95 and name N) (segid 3A4 and resid 98 and name N)	4.81	0.15	0.14
	assign (segid 3A4 and resid 95 and name N) (segid 3A4 and resid 99 and name N)	6.33	0.56	0.56
	assign (segid 3A4 and resid 95 and name N) (segid 3A4 and resid 100 and name N)	5.29	0.58	0.59
	assign (segid 3A4 and resid 95 and name O) (segid 3A4 and resid 101 and name N)	7.13	0.28	0.28
20	assign (segid 3A4 and resid 95 and name O) (segid 3A4 and resid 95 and name CB)	3.26	0.06	0.06
	assign (segid 3A4 and resid 95 and name O) (segid 3A4 and resid 96 and name C)	2.98	0.11	0.10
	assign (segid 3A4 and resid 95 and name O) (segid 3A4 and resid 96 and name CA)	2.77	0.04	0.04
	assign (segid 3A4 and resid 95 and name O) (segid 3A4 and resid 96 and name CB)	4.24	0.04	0.04
	assign (segid 3A4 and resid 95 and name O) (segid 3A4 and resid 96 and name N)	2.26	0.02	0.01
25	assign (segid 3A4 and resid 95 and name O) (segid 3A4 and resid 96 and name O)	3.54	0.20	0.19
	assign (segid 3A4 and resid 95 and name O) (segid 3A4 and resid 97 and name C)	4.00	0.12	0.13
	assign (segid 3A4 and resid 95 and name O) (segid 3A4 and resid 97 and name CA)	4.27	0.13	0.13
	assign (segid 3A4 and resid 95 and name O) (segid 3A4 and resid 97 and name CB)	5.27	0.14	0.14
	assign (segid 3A4 and resid 95 and name O) (segid 3A4 and resid 97 and name N)	3.34	0.16	0.16
30	assign (segid 3A4 and resid 95 and name O) (segid 3A4 and resid 97 and name O)	4.97	0.14	0.13
	assign (segid 3A4 and resid 95 and name O) (segid 3A4 and resid 98 and name C)	3.94	0.37	0.36
	assign (segid 3A4 and resid 95 and name O) (segid 3A4 and resid 98 and name CA)	3.74	0.17	0.18
	assign (segid 3A4 and resid 95 and name O) (segid 3A4 and resid 98 and name CB)	3.62	0.23	0.24
	assign (segid 3A4 and resid 95 and name O) (segid 3A4 and resid 98 and name N)	3.21	0.18	0.19
35	assign (segid 3A4 and resid 95 and name O) (segid 3A4 and resid 98 and name O)	5.10	0.36	0.37
	assign (segid 3A4 and resid 95 and name O) (segid 3A4 and resid 99 and name C)	5.31	0.69	0.68
	assign (segid 3A4 and resid 95 and name O) (segid 3A4 and resid 99 and name CA)	4.19	0.76	0.75
	assign (segid 3A4 and resid 95 and name O) (segid 3A4 and resid 99 and name CB)	3.93	0.90	0.89
	assign (segid 3A4 and resid 95 and name O) (segid 3A4 and resid 99 and name N)	3.23	0.60	0.60
40	assign (segid 3A4 and resid 95 and name O) (segid 3A4 and resid 100 and name C)	6.41	0.44	0.45
	assign (segid 3A4 and resid 96 and name C) (segid 3A4 and resid 100 and name CA)	5.32	0.52	0.52
	assign (segid 3A4 and resid 96 and name C) (segid 3A4 and resid 100 and name CB)	4.95	0.47	0.47
	assign (segid 3A4 and resid 96 and name C) (segid 3A4 and resid 100 and name N)	4.41	0.54	0.53
45	assign (segid 3A4 and resid 96 and name C) (segid 3A4 and resid 101 and name N)	6.33	0.33	0.33
	assign (segid 3A4 and resid 96 and name C) (segid 3A4 and resid 96 and name CB)	2.50	0.02	0.02
	assign (segid 3A4 and resid 96 and name C) (segid 3A4 and resid 96 and name O)	1.24	0.01	0.00
	assign (segid 3A4 and resid 96 and name C) (segid 3A4 and resid 97 and name C)	3.10	0.08	0.09
	assign (segid 3A4 and resid 96 and name C) (segid 3A4 and resid 97 and name CA)	2.44	0.01	0.02
	assign (segid 3A4 and resid 96 and name C) (segid 3A4 and resid 97 and name CB)	3.73	0.04	0.04
50	assign (segid 3A4 and resid 96 and name C) (segid 3A4 and resid 97 and name N)	1.34	0.01	0.01
	assign (segid 3A4 and resid 96 and name C) (segid 3A4 and resid 97 and name O)	3.98	0.16	0.15
	assign (segid 3A4 and resid 96 and name C) (segid 3A4 and resid 98 and name C)	4.72	0.26	0.26
	assign (segid 3A4 and resid 96 and name C) (segid 3A4 and resid 98 and name CA)	4.60	0.09	0.09
	assign (segid 3A4 and resid 96 and name C) (segid 3A4 and resid 98 and name CB)	5.34	0.09	0.09
55	assign (segid 3A4 and resid 96 and name C) (segid 3A4 and resid 98 and name N)	3.40	0.08	0.07
	assign (segid 3A4 and resid 96 and name C) (segid 3A4 and resid 98 and name O)	5.77	0.27	0.27
	assign (segid 3A4 and resid 96 and name C) (segid 3A4 and resid 99 and name C)	5.13	0.54	0.55
	assign (segid 3A4 and resid 96 and name C) (segid 3A4 and resid 99 and name CA)	4.79	0.51	0.52
	assign (segid 3A4 and resid 96 and name C) (segid 3A4 and resid 99 and name CB)	4.57	0.58	0.57
60	assign (segid 3A4 and resid 96 and name C) (segid 3A4 and resid 99 and name N)	4.04	0.39	0.38
	assign (segid 3A4 and resid 96 and name C) (segid 3A4 and resid 99 and name O)	6.34	0.55	0.55
	assign (segid 3A4 and resid 96 and name C) (segid 3A4 and resid 100 and name CA)	6.52	0.61	0.61
	assign (segid 3A4 and resid 96 and name CA) (segid 3A4 and resid 100 and name N)	6.26	0.55	0.54
	assign (segid 3A4 and resid 96 and name CA) (segid 3A4 and resid 100 and name CB)	5.52	0.63	0.63
65	assign (segid 3A4 and resid 96 and name CA) (segid 3A4 and resid 101 and name CA)	8.96	0.27	0.27
	assign (segid 3A4 and resid 96 and name CA) (segid 3A4 and resid 101 and name CB)	9.04	0.23	0.22
	assign (segid 3A4 and resid 96 and name CA) (segid 3A4 and resid 102 and name CA)	10.11	0.45	0.46
	assign (segid 3A4 and resid 96 and name CA) (segid 3A4 and resid 102 and name CB)	10.92	0.61	0.61
	assign (segid 3A4 and resid 96 and name CA) (segid 3A4 and resid 103 and name CB)	10.20	0.66	0.66
70	assign (segid 3A4 and resid 96 and name CA) (segid 3A4 and resid 104 and name CA)	12.70	0.51	0.51
	assign (segid 3A4 and resid 96 and name CA) (segid 3A4 and resid 104 and name CB)	12.32	0.50	0.50
	assign (segid 3A4 and resid 96 and name CA) (segid 3A4 and resid 105 and name CA)	14.56	0.40	0.40
	assign (segid 3A4 and resid 96 and name CA) (segid 3A4 and resid 105 and name CB)	14.17	0.40	0.39
	assign (segid 3A4 and resid 96 and name CA) (segid 3A4 and resid 106 and name CA)	15.67	0.60	0.59
75	assign (segid 3A4 and resid 96 and name CA) (segid 3A4 and resid 106 and name CB)	14.97	0.66	0.65
	assign (segid 3A4 and resid 96 and name CA) (segid 3A4 and resid 107 and name CA)	16.85	0.69	0.68
	assign (segid 3A4 and resid 96 and name CA) (segid 3A4 and resid 107 and name CB)	16.18	0.69	0.68
	assign (segid 3A4 and resid 96 and name CA) (segid 3A4 and resid 108 and name CB)	18.33	0.51	0.50
	assign (segid 3A4 and resid 96 and name CA) (segid 3A4 and resid 128 and name CA)	16.60	1.72	1.72
80	assign (segid 3A4 and resid 96 and name CA) (segid 3A4 and resid 129 and name CA)	14.55	0.85	0.85
	assign (segid 3A4 and resid 96 and name CA) (segid 3A4 and resid 129 and name CB)	14.85	0.94	0.94
	assign (segid 3A4 and resid 96 and name CA) (segid 3A4 and resid 130 and name CA)	15.26	0.62	0.63

	assign (segid 3A4 and resid 96 and name CA) (segid 3A4 and resid 130 and name CB)	16.41	0.66	0.67
	assign (segid 3A4 and resid 96 and name CA) (segid 3A4 and resid 131 and name CA)	15.54	1.40	1.39
	assign (segid 3A4 and resid 96 and name CA) (segid 3A4 and resid 131 and name CB)	16.32	1.96	1.96
	assign (segid 3A4 and resid 96 and name CA) (segid 3A4 and resid 132 and name CA)	13.01	1.58	1.58
5	assign (segid 3A4 and resid 96 and name CA) (segid 3A4 and resid 132 and name CB)	12.73	1.55	1.55
	assign (segid 3A4 and resid 96 and name CA) (segid 3A4 and resid 133 and name CA)	12.03	0.53	0.53
	assign (segid 3A4 and resid 96 and name CA) (segid 3A4 and resid 133 and name CB)	12.20	1.20	1.21
	assign (segid 3A4 and resid 96 and name CA) (segid 3A4 and resid 134 and name CA)	14.12	0.45	0.44
	assign (segid 3A4 and resid 96 and name CA) (segid 3A4 and resid 135 and name CA)	13.90	2.03	2.04
	assign (segid 3A4 and resid 96 and name CA) (segid 3A4 and resid 135 and name CB)	13.94	2.69	2.69
10	assign (segid 3A4 and resid 96 and name CA) (segid 3A4 and resid 136 and name CA)	11.74	1.17	1.18
	assign (segid 3A4 and resid 96 and name CA) (segid 3A4 and resid 136 and name CB)	10.83	0.84	0.83
	assign (segid 3A4 and resid 96 and name CA) (segid 3A4 and resid 137 and name CA)	12.90	0.93	0.94
	assign (segid 3A4 and resid 96 and name CA) (segid 3A4 and resid 138 and name CA)	15.70	0.99	0.99
	assign (segid 3A4 and resid 96 and name CA) (segid 3A4 and resid 138 and name CB)	16.67	0.95	0.95
15	assign (segid 3A4 and resid 96 and name CA) (segid 3A4 and resid 139 and name CA)	14.99	1.78	1.77
	assign (segid 3A4 and resid 96 and name CA) (segid 3A4 and resid 140 and name CA)	16.93	1.81	1.81
	assign (segid 3A4 and resid 96 and name CA) (segid 3A4 and resid 140 and name CB)	17.63	1.43	1.44
	assign (segid 3A4 and resid 96 and name CA) (segid 3A4 and resid 219 and name CA)	14.08	1.74	1.74
20	assign (segid 3A4 and resid 96 and name CA) (segid 3A4 and resid 219 and name CB)	14.45	1.72	1.71
	assign (segid 3A4 and resid 96 and name CA) (segid 3A4 and resid 220 and name CA)	15.97	1.74	1.75
	assign (segid 3A4 and resid 96 and name CA) (segid 3A4 and resid 220 and name CB)	15.86	1.72	1.72
	assign (segid 3A4 and resid 96 and name CA) (segid 3A4 and resid 259 and name CA)	18.47	0.43	0.44
	assign (segid 3A4 and resid 96 and name CA) (segid 3A4 and resid 259 and name CB)	17.13	0.50	0.49
25	assign (segid 3A4 and resid 96 and name CA) (segid 3A4 and resid 305 and name CA)	17.74	1.30	1.29
	assign (segid 3A4 and resid 96 and name CA) (segid 3A4 and resid 306 and name CA)	18.53	0.85	0.85
	assign (segid 3A4 and resid 96 and name CA) (segid 3A4 and resid 393 and name CA)	16.88	1.09	1.09
	assign (segid 3A4 and resid 96 and name CA) (segid 3A4 and resid 394 and name CA)	17.53	0.99	0.99
	assign (segid 3A4 and resid 96 and name CA) (segid 3A4 and resid 395 and name CA)	14.46	1.12	1.12
	assign (segid 3A4 and resid 96 and name CA) (segid 3A4 and resid 396 and name CA)	12.29	0.85	0.84
30	assign (segid 3A4 and resid 96 and name CA) (segid 3A4 and resid 396 and name CB)	12.41	1.04	1.03
	assign (segid 3A4 and resid 96 and name CA) (segid 3A4 and resid 397 and name CA)	14.72	0.48	0.48
	assign (segid 3A4 and resid 96 and name CA) (segid 3A4 and resid 397 and name CB)	16.16	0.52	0.52
	assign (segid 3A4 and resid 96 and name CA) (segid 3A4 and resid 398 and name CA)	14.75	0.39	0.39
35	assign (segid 3A4 and resid 96 and name CA) (segid 3A4 and resid 398 and name CB)	15.34	0.56	0.56
	assign (segid 3A4 and resid 96 and name CA) (segid 3A4 and resid 399 and name CA)	11.16	0.38	0.38
	assign (segid 3A4 and resid 96 and name CA) (segid 3A4 and resid 399 and name CB)	10.13	0.51	0.52
	assign (segid 3A4 and resid 96 and name CA) (segid 3A4 and resid 400 and name CA)	11.36	0.60	0.59
	assign (segid 3A4 and resid 96 and name CA) (segid 3A4 and resid 400 and name CB)	11.90	0.56	0.55
40	assign (segid 3A4 and resid 96 and name CA) (segid 3A4 and resid 401 and name CA)	14.55	0.66	0.66
	assign (segid 3A4 and resid 96 and name CA) (segid 3A4 and resid 402 and name CA)	13.78	0.78	0.77
	assign (segid 3A4 and resid 96 and name CA) (segid 3A4 and resid 402 and name CB)	13.51	0.66	0.67
	assign (segid 3A4 and resid 96 and name CA) (segid 3A4 and resid 403 and name CA)	10.96	1.15	1.16
	assign (segid 3A4 and resid 96 and name CA) (segid 3A4 and resid 403 and name CB)	9.62	1.14	1.13
45	assign (segid 3A4 and resid 96 and name CA) (segid 3A4 and resid 404 and name CA)	13.26	1.28	1.28
	assign (segid 3A4 and resid 96 and name CA) (segid 3A4 and resid 404 and name CB)	13.88	1.16	1.16
	assign (segid 3A4 and resid 96 and name CA) (segid 3A4 and resid 405 and name CA)	16.23	1.30	1.31
	assign (segid 3A4 and resid 96 and name CA) (segid 3A4 and resid 406 and name CA)	15.12	1.56	1.57
	assign (segid 3A4 and resid 96 and name CA) (segid 3A4 and resid 407 and name CA)	14.22	1.77	1.78
	assign (segid 3A4 and resid 96 and name CA) (segid 3A4 and resid 407 and name CB)	13.03	1.81	1.80
50	assign (segid 3A4 and resid 96 and name CA) (segid 3A4 and resid 96 and name C)	1.52	0.02	0.02
	assign (segid 3A4 and resid 96 and name CA) (segid 3A4 and resid 96 and name CB)	1.52	0.01	0.01
	assign (segid 3A4 and resid 96 and name CA) (segid 3A4 and resid 96 and name O)	2.39	0.01	0.01
	assign (segid 3A4 and resid 96 and name CA) (segid 3A4 and resid 97 and name C)	4.45	0.07	0.07
	assign (segid 3A4 and resid 96 and name CA) (segid 3A4 and resid 97 and name CA)	3.81	0.02	0.03
55	assign (segid 3A4 and resid 96 and name CA) (segid 3A4 and resid 97 and name CB)	4.89	0.06	0.06
	assign (segid 3A4 and resid 96 and name CA) (segid 3A4 and resid 97 and name N)	2.45	0.02	0.02
	assign (segid 3A4 and resid 96 and name CA) (segid 3A4 and resid 97 and name O)	5.41	0.14	0.13
	assign (segid 3A4 and resid 96 and name CA) (segid 3A4 and resid 98 and name C)	5.65	0.28	0.29
	assign (segid 3A4 and resid 96 and name CA) (segid 3A4 and resid 98 and name CA)	5.54	0.10	0.10
60	assign (segid 3A4 and resid 96 and name CA) (segid 3A4 and resid 98 and name CB)	5.94	0.15	0.14
	assign (segid 3A4 and resid 96 and name CA) (segid 3A4 and resid 98 and name N)	4.43	0.09	0.10
	assign (segid 3A4 and resid 96 and name CA) (segid 3A4 and resid 98 and name O)	6.77	0.31	0.30
	assign (segid 3A4 and resid 96 and name CA) (segid 3A4 and resid 99 and name C)	6.03	0.67	0.67
	assign (segid 3A4 and resid 96 and name CA) (segid 3A4 and resid 99 and name CA)	5.44	0.66	0.65
65	assign (segid 3A4 and resid 96 and name CA) (segid 3A4 and resid 99 and name CB)	4.83	0.79	0.80
	assign (segid 3A4 and resid 96 and name CA) (segid 3A4 and resid 99 and name N)	4.80	0.46	0.46
	assign (segid 3A4 and resid 96 and name CB) (segid 3A4 and resid 100 and name CA)	7.35	0.63	0.63
	assign (segid 3A4 and resid 96 and name CB) (segid 3A4 and resid 100 and name CB)	6.84	0.58	0.59
70	assign (segid 3A4 and resid 96 and name CB) (segid 3A4 and resid 101 and name CA)	10.02	0.29	0.28
	assign (segid 3A4 and resid 96 and name CB) (segid 3A4 and resid 101 and name CB)	10.13	0.22	0.23
	assign (segid 3A4 and resid 96 and name CB) (segid 3A4 and resid 102 and name CA)	11.41	0.46	0.46
	assign (segid 3A4 and resid 96 and name CB) (segid 3A4 and resid 103 and name CA)	11.94	0.62	0.62
	assign (segid 3A4 and resid 96 and name CB) (segid 3A4 and resid 103 and name CB)	11.09	0.66	0.67
	assign (segid 3A4 and resid 96 and name CB) (segid 3A4 and resid 104 and name CA)	13.57	0.54	0.54
75	assign (segid 3A4 and resid 96 and name CB) (segid 3A4 and resid 104 and name CB)	13.13	0.53	0.53
	assign (segid 3A4 and resid 96 and name CB) (segid 3A4 and resid 105 and name CA)	15.68	0.42	0.42
	assign (segid 3A4 and resid 96 and name CB) (segid 3A4 and resid 105 and name CB)	15.37	0.42	0.42
	assign (segid 3A4 and resid 96 and name CB) (segid 3A4 and resid 106 and name CA)	16.81	0.60	0.61
	assign (segid 3A4 and resid 96 and name CB) (segid 3A4 and resid 106 and name CB)	16.12	0.66	0.66
80	assign (segid 3A4 and resid 96 and name CB) (segid 3A4 and resid 107 and name CA)	17.75	0.71	0.71
	assign (segid 3A4 and resid 96 and name CB) (segid 3A4 and resid 107 and name CB)	16.98	0.72	0.72
	assign (segid 3A4 and resid 96 and name CB) (segid 3A4 and resid 129 and name CA)	15.73	0.73	0.73

	assign (segid 3A4 and resid 96 and name CB) (segid 3A4 and resid 129 and name CB)	16.10	0.83	0.83
	assign (segid 3A4 and resid 96 and name CB) (segid 3A4 and resid 130 and name CA)	16.33	0.49	0.50
	assign (segid 3A4 and resid 96 and name CB) (segid 3A4 and resid 130 and name CB)	17.49	0.52	0.52
	assign (segid 3A4 and resid 96 and name CB) (segid 3A4 and resid 131 and name CA)	16.42	1.43	1.43
	assign (segid 3A4 and resid 96 and name CB) (segid 3A4 and resid 131 and name CB)	17.21	1.99	1.98
5	assign (segid 3A4 and resid 96 and name CB) (segid 3A4 and resid 132 and name CA)	13.86	1.51	1.51
	assign (segid 3A4 and resid 96 and name CB) (segid 3A4 and resid 132 and name CB)	13.65	1.44	1.43
	assign (segid 3A4 and resid 96 and name CB) (segid 3A4 and resid 133 and name CA)	12.85	0.45	0.46
	assign (segid 3A4 and resid 96 and name CB) (segid 3A4 and resid 133 and name CB)	13.12	1.10	1.10
	assign (segid 3A4 and resid 96 and name CB) (segid 3A4 and resid 134 and name CA)	14.74	0.64	0.65
10	assign (segid 3A4 and resid 96 and name CB) (segid 3A4 and resid 135 and name CA)	14.32	2.16	2.16
	assign (segid 3A4 and resid 96 and name CB) (segid 3A4 and resid 135 and name CB)	14.41	2.78	2.78
	assign (segid 3A4 and resid 96 and name CB) (segid 3A4 and resid 136 and name CA)	12.04	1.23	1.23
	assign (segid 3A4 and resid 96 and name CB) (segid 3A4 and resid 136 and name CB)	11.22	0.82	0.83
	assign (segid 3A4 and resid 96 and name CB) (segid 3A4 and resid 137 and name CA)	13.14	1.09	1.08
15	assign (segid 3A4 and resid 96 and name CB) (segid 3A4 and resid 138 and name CA)	15.79	1.26	1.26
	assign (segid 3A4 and resid 96 and name CB) (segid 3A4 and resid 138 and name CB)	16.83	1.23	1.23
	assign (segid 3A4 and resid 96 and name CB) (segid 3A4 and resid 139 and name CA)	14.89	1.95	1.94
	assign (segid 3A4 and resid 96 and name CB) (segid 3A4 and resid 139 and name CB)	17.01	1.96	1.96
	assign (segid 3A4 and resid 96 and name CB) (segid 3A4 and resid 140 and name CA)	13.79	1.95	1.95
20	assign (segid 3A4 and resid 96 and name CB) (segid 3A4 and resid 219 and name CB)	14.19	1.91	1.91
	assign (segid 3A4 and resid 96 and name CB) (segid 3A4 and resid 220 and name CA)	15.88	2.03	2.04
	assign (segid 3A4 and resid 96 and name CB) (segid 3A4 and resid 220 and name CB)	15.91	2.01	2.01
	assign (segid 3A4 and resid 96 and name CB) (segid 3A4 and resid 259 and name CB)	18.39	0.53	0.53
	assign (segid 3A4 and resid 96 and name CB) (segid 3A4 and resid 393 and name CA)	17.72	1.28	1.29
25	assign (segid 3A4 and resid 96 and name CB) (segid 3A4 and resid 395 and name CA)	15.41	1.22	1.22
	assign (segid 3A4 and resid 96 and name CB) (segid 3A4 and resid 396 and name CA)	13.31	0.93	0.94
	assign (segid 3A4 and resid 96 and name CB) (segid 3A4 and resid 396 and name CB)	13.35	1.15	1.14
	assign (segid 3A4 and resid 96 and name CB) (segid 3A4 and resid 397 and name CA)	15.92	0.55	0.56
	assign (segid 3A4 and resid 96 and name CB) (segid 3A4 and resid 397 and name CB)	17.34	0.62	0.63
30	assign (segid 3A4 and resid 96 and name CB) (segid 3A4 and resid 398 and name CA)	16.02	0.44	0.43
	assign (segid 3A4 and resid 96 and name CB) (segid 3A4 and resid 398 and name CB)	16.56	0.61	0.61
	assign (segid 3A4 and resid 96 and name CB) (segid 3A4 and resid 399 and name CA)	12.46	0.38	0.37
	assign (segid 3A4 and resid 96 and name CB) (segid 3A4 and resid 399 and name CB)	11.37	0.51	0.51
35	assign (segid 3A4 and resid 96 and name CB) (segid 3A4 and resid 400 and name CA)	12.76	0.51	0.51
	assign (segid 3A4 and resid 96 and name CB) (segid 3A4 and resid 400 and name CB)	13.25	0.46	0.45
	assign (segid 3A4 and resid 96 and name CB) (segid 3A4 and resid 401 and name CA)	16.00	0.59	0.58
	assign (segid 3A4 and resid 96 and name CB) (segid 3A4 and resid 402 and name CA)	15.21	0.77	0.76
	assign (segid 3A4 and resid 96 and name CB) (segid 3A4 and resid 402 and name CB)	14.89	0.68	0.68
40	assign (segid 3A4 and resid 96 and name CB) (segid 3A4 and resid 403 and name CA)	12.42	1.14	1.14
	assign (segid 3A4 and resid 96 and name CB) (segid 3A4 and resid 403 and name CB)	11.09	1.11	1.11
	assign (segid 3A4 and resid 96 and name CB) (segid 3A4 and resid 404 and name CA)	14.72	1.23	1.23
	assign (segid 3A4 and resid 96 and name CB) (segid 3A4 and resid 404 and name CB)	15.33	1.09	1.10
	assign (segid 3A4 and resid 96 and name CB) (segid 3A4 and resid 407 and name CB)	14.34	1.84	1.84
45	assign (segid 3A4 and resid 96 and name CB) (segid 3A4 and resid 97 and name C)	5.52	0.10	0.09
	assign (segid 3A4 and resid 96 and name CB) (segid 3A4 and resid 97 and name CA)	4.54	0.07	0.08
	assign (segid 3A4 and resid 96 and name CB) (segid 3A4 and resid 97 and name CB)	5.43	0.12	0.12
	assign (segid 3A4 and resid 96 and name CB) (segid 3A4 and resid 97 and name N)	3.22	0.09	0.09
	assign (segid 3A4 and resid 96 and name CB) (segid 3A4 and resid 97 and name O)	6.43	0.16	0.16
	assign (segid 3A4 and resid 96 and name CB) (segid 3A4 and resid 98 and name C)	7.07	0.28	0.27
50	assign (segid 3A4 and resid 96 and name CB) (segid 3A4 and resid 98 and name CA)	6.92	0.09	0.08
	assign (segid 3A4 and resid 96 and name CB) (segid 3A4 and resid 98 and name CB)	7.37	0.11	0.11
	assign (segid 3A4 and resid 96 and name CB) (segid 3A4 and resid 98 and name N)	5.70	0.07	0.08
	assign (segid 3A4 and resid 96 and name CB) (segid 3A4 and resid 99 and name CA)	6.77	0.61	0.62
	assign (segid 3A4 and resid 96 and name CB) (segid 3A4 and resid 99 and name CB)	6.08	0.75	0.74
55	assign (segid 3A4 and resid 96 and name CB) (segid 3A4 and resid 99 and name N)	6.22	0.43	0.43
	assign (segid 3A4 and resid 96 and name CB) (segid 3A4 and resid 99 and name O)	6.39	0.56	0.56
	assign (segid 3A4 and resid 96 and name N) (segid 3A4 and resid 96 and name C)	2.46	0.03	0.03
	assign (segid 3A4 and resid 96 and name N) (segid 3A4 and resid 96 and name CA)	1.47	0.01	0.01
60	assign (segid 3A4 and resid 96 and name N) (segid 3A4 and resid 96 and name CB)	2.43	0.03	0.03
	assign (segid 3A4 and resid 96 and name N) (segid 3A4 and resid 96 and name O)	3.52	0.05	0.05
	assign (segid 3A4 and resid 96 and name N) (segid 3A4 and resid 97 and name C)	4.70	0.05	0.06
	assign (segid 3A4 and resid 96 and name N) (segid 3A4 and resid 97 and name CA)	4.18	0.06	0.07
	assign (segid 3A4 and resid 96 and name N) (segid 3A4 and resid 97 and name CB)	4.97	0.13	0.14
	assign (segid 3A4 and resid 96 and name N) (segid 3A4 and resid 97 and name N)	2.79	0.08	0.09
65	assign (segid 3A4 and resid 96 and name N) (segid 3A4 and resid 97 and name O)	5.82	0.11	0.10
	assign (segid 3A4 and resid 96 and name N) (segid 3A4 and resid 98 and name C)	5.77	0.31	0.30
	assign (segid 3A4 and resid 96 and name N) (segid 3A4 and resid 98 and name CA)	5.38	0.09	0.09
	assign (segid 3A4 and resid 96 and name N) (segid 3A4 and resid 98 and name CB)	5.45	0.11	0.11
	assign (segid 3A4 and resid 96 and name N) (segid 3A4 and resid 98 and name N)	4.34	0.08	0.08
70	assign (segid 3A4 and resid 96 and name N) (segid 3A4 and resid 98 and name O)	6.95	0.29	0.30
	assign (segid 3A4 and resid 96 and name N) (segid 3A4 and resid 99 and name CA)	5.93	0.69	0.69
	assign (segid 3A4 and resid 96 and name N) (segid 3A4 and resid 99 and name CB)	5.42	0.87	0.86
	assign (segid 3A4 and resid 96 and name N) (segid 3A4 and resid 99 and name N)	5.06	0.53	0.52
	assign (segid 3A4 and resid 96 and name N) (segid 3A4 and resid 100 and name C)	5.43	0.63	0.63
75	assign (segid 3A4 and resid 96 and name O) (segid 3A4 and resid 100 and name CA)	4.23	0.68	0.68
	assign (segid 3A4 and resid 96 and name O) (segid 3A4 and resid 100 and name CB)	3.94	0.60	0.60
	assign (segid 3A4 and resid 96 and name O) (segid 3A4 and resid 100 and name N)	3.37	0.69	0.69
	assign (segid 3A4 and resid 96 and name O) (segid 3A4 and resid 101 and name N)	5.52	0.53	0.53
	assign (segid 3A4 and resid 96 and name O) (segid 3A4 and resid 96 and name CB)	3.25	0.10	0.10
80	assign (segid 3A4 and resid 96 and name O) (segid 3A4 and resid 97 and name C)	3.13	0.16	0.16
	assign (segid 3A4 and resid 96 and name O) (segid 3A4 and resid 97 and name CA)	2.77	0.02	0.03
	assign (segid 3A4 and resid 96 and name O) (segid 3A4 and resid 97 and name CB)	4.24	0.03	0.02

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	assign (segid 3A4 and resid 96 and name O) (segid 3A4 and resid 97 and name N)	2.25	0.01	0.01
	assign (segid 3A4 and resid 96 and name O) (segid 3A4 and resid 97 and name O)	3.66	0.27	0.26
	assign (segid 3A4 and resid 96 and name O) (segid 3A4 and resid 98 and name C)	4.41	0.37	0.37
	assign (segid 3A4 and resid 96 and name O) (segid 3A4 and resid 98 and name CA)	4.64	0.18	0.19
5	assign (segid 3A4 and resid 96 and name O) (segid 3A4 and resid 98 and name CB)	5.58	0.11	0.11
	assign (segid 3A4 and resid 96 and name O) (segid 3A4 and resid 98 and name N)	3.64	0.12	0.11
	assign (segid 3A4 and resid 96 and name O) (segid 3A4 and resid 98 and name O)	5.30	0.41	0.42
	assign (segid 3A4 and resid 96 and name O) (segid 3A4 and resid 99 and name C)	4.19	0.68	0.68
	assign (segid 3A4 and resid 96 and name O) (segid 3A4 and resid 99 and name CA)	4.11	0.60	0.60
10	assign (segid 3A4 and resid 96 and name O) (segid 3A4 and resid 99 and name CB)	3.94	0.58	0.57
	assign (segid 3A4 and resid 96 and name O) (segid 3A4 and resid 99 and name N)	3.63	0.45	0.45
	assign (segid 3A4 and resid 96 and name O) (segid 3A4 and resid 99 and name O)	5.36	0.70	0.70
	assign (segid 3A4 and resid 97 and name C) (segid 3A4 and resid 100 and name C)	4.93	0.16	0.15
	assign (segid 3A4 and resid 97 and name C) (segid 3A4 and resid 100 and name CA)	4.51	0.09	0.09
15	assign (segid 3A4 and resid 97 and name C) (segid 3A4 and resid 100 and name CB)	4.31	0.15	0.14
	assign (segid 3A4 and resid 97 and name C) (segid 3A4 and resid 100 and name N)	3.76	0.06	0.05
	assign (segid 3A4 and resid 97 and name C) (segid 3A4 and resid 100 and name O)	6.15	0.14	0.15
	assign (segid 3A4 and resid 97 and name C) (segid 3A4 and resid 101 and name C)	6.25	0.19	0.18
20	assign (segid 3A4 and resid 97 and name C) (segid 3A4 and resid 101 and name CA)	5.25	0.26	0.25
	assign (segid 3A4 and resid 97 and name C) (segid 3A4 and resid 101 and name CB)	4.93	0.33	0.32
	assign (segid 3A4 and resid 97 and name C) (segid 3A4 and resid 101 and name CG)	6.32	0.34	0.33
	assign (segid 3A4 and resid 97 and name C) (segid 3A4 and resid 101 and name N)	4.27	0.21	0.21
	assign (segid 3A4 and resid 97 and name C) (segid 3A4 and resid 101 and name O)	7.43	0.20	0.19
	assign (segid 3A4 and resid 97 and name C) (segid 3A4 and resid 102 and name CA)	7.25	0.11	0.10
25	assign (segid 3A4 and resid 97 and name C) (segid 3A4 and resid 102 and name N)	6.02	0.14	0.13
	assign (segid 3A4 and resid 97 and name C) (segid 3A4 and resid 97 and name CB)	2.46	0.05	0.04
	assign (segid 3A4 and resid 97 and name C) (segid 3A4 and resid 97 and name O)	1.23	0.01	0.01
	assign (segid 3A4 and resid 97 and name C) (segid 3A4 and resid 98 and name C)	2.98	0.02	0.01
30	assign (segid 3A4 and resid 97 and name C) (segid 3A4 and resid 98 and name CA)	2.43	0.01	0.01
	assign (segid 3A4 and resid 97 and name C) (segid 3A4 and resid 98 and name CB)	3.73	0.03	0.03
	assign (segid 3A4 and resid 97 and name C) (segid 3A4 and resid 98 and name N)	1.33	0.00	0.00
	assign (segid 3A4 and resid 97 and name C) (segid 3A4 and resid 98 and name O)	3.77	0.06	0.07
	assign (segid 3A4 and resid 97 and name C) (segid 3A4 and resid 99 and name C)	4.50	0.04	0.05
35	assign (segid 3A4 and resid 97 and name C) (segid 3A4 and resid 99 and name CA)	4.43	0.06	0.06
	assign (segid 3A4 and resid 97 and name C) (segid 3A4 and resid 99 and name CB)	5.15	0.06	0.06
	assign (segid 3A4 and resid 97 and name C) (segid 3A4 and resid 99 and name N)	3.25	0.07	0.07
	assign (segid 3A4 and resid 97 and name C) (segid 3A4 and resid 99 and name O)	5.58	0.07	0.07
	assign (segid 3A4 and resid 97 and name CA) (segid 3A4 and resid 100 and name C)	5.77	0.16	0.15
40	assign (segid 3A4 and resid 97 and name CA) (segid 3A4 and resid 100 and name CA)	5.10	0.12	0.12
	assign (segid 3A4 and resid 97 and name CA) (segid 3A4 and resid 100 and name CB)	4.49	0.18	0.17
	assign (segid 3A4 and resid 97 and name CA) (segid 3A4 and resid 100 and name N)	4.51	0.09	0.09
	assign (segid 3A4 and resid 97 and name CA) (segid 3A4 and resid 100 and name O)	6.97	0.15	0.14
	assign (segid 3A4 and resid 97 and name CA) (segid 3A4 and resid 101 and name C)	7.49	0.18	0.18
45	assign (segid 3A4 and resid 97 and name CA) (segid 3A4 and resid 101 and name CA)	6.36	0.25	0.26
	assign (segid 3A4 and resid 97 and name CA) (segid 3A4 and resid 101 and name CB)	6.11	0.33	0.34
	assign (segid 3A4 and resid 97 and name CA) (segid 3A4 and resid 101 and name N)	5.31	0.21	0.20
	assign (segid 3A4 and resid 97 and name CA) (segid 3A4 and resid 102 and name CA)	8.62	0.09	0.09
	assign (segid 3A4 and resid 97 and name CA) (segid 3A4 and resid 102 and name N)	7.36	0.13	0.13
50	assign (segid 3A4 and resid 97 and name CA) (segid 3A4 and resid 103 and name CA)	9.96	0.13	0.14
	assign (segid 3A4 and resid 97 and name CA) (segid 3A4 and resid 103 and name CB)	9.55	0.16	0.16
	assign (segid 3A4 and resid 97 and name CA) (segid 3A4 and resid 104 and name CA)	10.77	0.27	0.26
	assign (segid 3A4 and resid 97 and name CA) (segid 3A4 and resid 104 and name CB)	10.05	0.35	0.35
	assign (segid 3A4 and resid 97 and name CA) (segid 3A4 and resid 105 and name CA)	12.46	0.31	0.31
55	assign (segid 3A4 and resid 97 and name CA) (segid 3A4 and resid 105 and name CB)	12.02	0.36	0.37
	assign (segid 3A4 and resid 97 and name CA) (segid 3A4 and resid 106 and name CA)	14.35	0.16	0.17
	assign (segid 3A4 and resid 97 and name CA) (segid 3A4 and resid 106 and name CB)	13.99	0.13	0.13
	assign (segid 3A4 and resid 97 and name CA) (segid 3A4 and resid 107 and name CA)	15.50	0.16	0.16
	assign (segid 3A4 and resid 97 and name CA) (segid 3A4 and resid 107 and name CB)	14.83	0.15	0.15
60	assign (segid 3A4 and resid 97 and name CA) (segid 3A4 and resid 108 and name CA)	16.78	0.26	0.26
	assign (segid 3A4 and resid 97 and name CA) (segid 3A4 and resid 108 and name CB)	16.11	0.36	0.35
	assign (segid 3A4 and resid 97 and name CA) (segid 3A4 and resid 109 and name CA)	18.65	0.31	0.31
	assign (segid 3A4 and resid 97 and name CA) (segid 3A4 and resid 109 and name CB)	18.20	0.35	0.35
	assign (segid 3A4 and resid 97 and name CA) (segid 3A4 and resid 110 and name CB)	19.40	0.17	0.17
65	assign (segid 3A4 and resid 97 and name CA) (segid 3A4 and resid 125 and name CA)	16.50	0.79	0.79
	assign (segid 3A4 and resid 97 and name CA) (segid 3A4 and resid 125 and name CB)	16.99	0.79	0.79
	assign (segid 3A4 and resid 97 and name CA) (segid 3A4 and resid 126 and name CA)	16.64	0.48	0.47
	assign (segid 3A4 and resid 97 and name CA) (segid 3A4 and resid 127 and name CA)	16.28	1.27	1.26
	assign (segid 3A4 and resid 97 and name CA) (segid 3A4 and resid 127 and name CB)	17.26	1.57	1.57
	assign (segid 3A4 and resid 97 and name CA) (segid 3A4 and resid 128 and name CA)	13.50	1.48	1.48
70	assign (segid 3A4 and resid 97 and name CA) (segid 3A4 and resid 128 and name CB)	13.69	1.52	1.52
	assign (segid 3A4 and resid 97 and name CA) (segid 3A4 and resid 129 and name CA)	11.58	0.62	0.61
	assign (segid 3A4 and resid 97 and name CA) (segid 3A4 and resid 129 and name CB)	12.10	0.64	0.65
	assign (segid 3A4 and resid 97 and name CA) (segid 3A4 and resid 130 and name CA)	12.14	0.41	0.42
	assign (segid 3A4 and resid 97 and name CA) (segid 3A4 and resid 130 and name CB)	13.39	0.42	0.41
75	assign (segid 3A4 and resid 97 and name CA) (segid 3A4 and resid 131 and name CA)	12.09	1.47	1.47
	assign (segid 3A4 and resid 97 and name CA) (segid 3A4 and resid 131 and name CB)	12.88	1.97	1.98
	assign (segid 3A4 and resid 97 and name CA) (segid 3A4 and resid 132 and name CA)	9.45	1.52	1.53
	assign (segid 3A4 and resid 97 and name CA) (segid 3A4 and resid 132 and name CB)	9.29	1.38	1.37
	assign (segid 3A4 and resid 97 and name CA) (segid 3A4 and resid 133 and name CA)	8.63	0.47	0.48
80	assign (segid 3A4 and resid 97 and name CA) (segid 3A4 and resid 133 and name CB)	8.98	1.11	1.11
	assign (segid 3A4 and resid 97 and name CA) (segid 3A4 and resid 134 and name CA)	10.78	0.55	0.55
	assign (segid 3A4 and resid 97 and name CA) (segid 3A4 and resid 135 and name CA)	10.39	2.10	2.10
	assign (segid 3A4 and resid 97 and name CA) (segid 3A4 and resid 135 and name CB)	10.33	2.75	2.76

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	assign (segid 3A4 and resid 97 and name CB) (segid 3A4 and resid 403 and name CA)	11.77	0.36	0.36
	assign (segid 3A4 and resid 97 and name CB) (segid 3A4 and resid 403 and name CB)	10.23	0.36	0.36
	assign (segid 3A4 and resid 97 and name CB) (segid 3A4 and resid 404 and name CA)	13.08	0.41	0.41
	assign (segid 3A4 and resid 97 and name CB) (segid 3A4 and resid 404 and name CB)	13.21	0.44	0.49
5	assign (segid 3A4 and resid 97 and name CB) (segid 3A4 and resid 405 and name CA)	16.55	0.35	0.35
	assign (segid 3A4 and resid 97 and name CB) (segid 3A4 and resid 405 and name CB)	17.29	0.36	0.36
	assign (segid 3A4 and resid 97 and name CB) (segid 3A4 and resid 406 and name CA)	16.47	0.50	0.51
	assign (segid 3A4 and resid 97 and name CB) (segid 3A4 and resid 407 and name CA)	15.37	0.63	0.63
	assign (segid 3A4 and resid 97 and name CB) (segid 3A4 and resid 407 and name CB)	14.01	0.66	0.67
10	assign (segid 3A4 and resid 97 and name CB) (segid 3A4 and resid 408 and name CA)	17.68	0.55	0.54
	assign (segid 3A4 and resid 97 and name CB) (segid 3A4 and resid 408 and name CB)	17.84	0.50	0.50
	assign (segid 3A4 and resid 97 and name CB) (segid 3A4 and resid 98 and name C)	5.35	0.07	0.07
	assign (segid 3A4 and resid 97 and name CB) (segid 3A4 and resid 98 and name CA)	4.45	0.09	0.10
	assign (segid 3A4 and resid 97 and name CB) (segid 3A4 and resid 98 and name CB)	5.41	0.16	0.15
15	assign (segid 3A4 and resid 97 and name CB) (segid 3A4 and resid 98 and name N)	3.16	0.11	0.10
	assign (segid 3A4 and resid 97 and name CB) (segid 3A4 and resid 98 and name O)	6.13	0.11	0.11
	assign (segid 3A4 and resid 97 and name CB) (segid 3A4 and resid 99 and name C)	6.78	0.04	0.04
	assign (segid 3A4 and resid 97 and name CB) (segid 3A4 and resid 99 and name CA)	6.75	0.08	0.09
	assign (segid 3A4 and resid 97 and name CB) (segid 3A4 and resid 99 and name CB)	7.25	0.13	0.12
20	assign (segid 3A4 and resid 97 and name CB) (segid 3A4 and resid 99 and name N)	5.58	0.11	0.11
	assign (segid 3A4 and resid 97 and name CB) (segid 3A4 and resid 99 and name O)	7.85	0.08	0.09
	assign (segid 3A4 and resid 97 and name N) (segid 3A4 and resid 100 and name C)	6.61	0.22	0.22
	assign (segid 3A4 and resid 97 and name N) (segid 3A4 and resid 100 and name CA)	5.72	0.28	0.28
	assign (segid 3A4 and resid 97 and name N) (segid 3A4 and resid 100 and name CB)	5.21	0.29	0.29
25	assign (segid 3A4 and resid 97 and name N) (segid 3A4 and resid 100 and name N)	4.91	0.29	0.29
	assign (segid 3A4 and resid 97 and name N) (segid 3A4 and resid 101 and name CA)	7.45	0.21	0.21
	assign (segid 3A4 and resid 97 and name N) (segid 3A4 and resid 101 and name N)	6.30	0.20	0.19
	assign (segid 3A4 and resid 97 and name N) (segid 3A4 and resid 97 and name C)	2.46	0.01	0.01
	assign (segid 3A4 and resid 97 and name N) (segid 3A4 and resid 97 and name CA)	1.45	0.01	0.01
30	assign (segid 3A4 and resid 97 and name N) (segid 3A4 and resid 97 and name CB)	2.48	0.04	0.03
	assign (segid 3A4 and resid 97 and name N) (segid 3A4 and resid 97 and name O)	3.50	0.05	0.05
	assign (segid 3A4 and resid 97 and name N) (segid 3A4 and resid 98 and name C)	4.73	0.09	0.10
	assign (segid 3A4 and resid 97 and name N) (segid 3A4 and resid 98 and name CA)	4.23	0.05	0.05
	assign (segid 3A4 and resid 97 and name N) (segid 3A4 and resid 98 and name CB)	5.00	0.08	0.09
35	assign (segid 3A4 and resid 97 and name N) (segid 3A4 and resid 98 and name N)	2.82	0.06	0.06
	assign (segid 3A4 and resid 97 and name N) (segid 3A4 and resid 98 and name O)	5.78	0.09	0.08
	assign (segid 3A4 and resid 97 and name N) (segid 3A4 and resid 99 and name C)	5.71	0.29	0.30
	assign (segid 3A4 and resid 97 and name N) (segid 3A4 and resid 99 and name CA)	5.42	0.31	0.30
	assign (segid 3A4 and resid 97 and name N) (segid 3A4 and resid 99 and name CB)	5.47	0.37	0.38
40	assign (segid 3A4 and resid 97 and name N) (segid 3A4 and resid 99 and name N)	4.39	0.24	0.23
	assign (segid 3A4 and resid 97 and name N) (segid 3A4 and resid 99 and name O)	6.92	0.29	0.29
	assign (segid 3A4 and resid 97 and name O) (segid 3A4 and resid 100 and name C)	3.88	0.18	0.19
	assign (segid 3A4 and resid 97 and name O) (segid 3A4 and resid 100 and name CA)	3.72	0.15	0.15
	assign (segid 3A4 and resid 97 and name O) (segid 3A4 and resid 100 and name CB)	3.57	0.18	0.19
45	assign (segid 3A4 and resid 97 and name O) (segid 3A4 and resid 100 and name N)	3.23	0.15	0.15
	assign (segid 3A4 and resid 97 and name O) (segid 3A4 and resid 100 and name O)	5.09	0.19	0.18
	assign (segid 3A4 and resid 97 and name O) (segid 3A4 and resid 101 and name C)	5.17	0.19	0.20
	assign (segid 3A4 and resid 97 and name O) (segid 3A4 and resid 101 and name CA)	4.09	0.25	0.25
	assign (segid 3A4 and resid 97 and name O) (segid 3A4 and resid 101 and name CB)	3.86	0.28	0.29
	assign (segid 3A4 and resid 97 and name O) (segid 3A4 and resid 101 and name CG)	5.30	0.29	0.29
50	assign (segid 3A4 and resid 97 and name O) (segid 3A4 and resid 101 and name N)	3.13	0.22	0.23
	assign (segid 3A4 and resid 97 and name O) (segid 3A4 and resid 101 and name O)	6.33	0.21	0.21
	assign (segid 3A4 and resid 97 and name O) (segid 3A4 and resid 102 and name C)	7.29	0.16	0.16
	assign (segid 3A4 and resid 97 and name O) (segid 3A4 and resid 102 and name CA)	6.42	0.13	0.13
	assign (segid 3A4 and resid 97 and name O) (segid 3A4 and resid 102 and name N)	5.10	0.15	0.16
55	assign (segid 3A4 and resid 97 and name O) (segid 3A4 and resid 103 and name N)	6.95	0.20	0.20
	assign (segid 3A4 and resid 97 and name O) (segid 3A4 and resid 97 and name CB)	3.16	0.10	0.11
	assign (segid 3A4 and resid 97 and name O) (segid 3A4 and resid 98 and name C)	2.93	0.06	0.06
	assign (segid 3A4 and resid 97 and name O) (segid 3A4 and resid 98 and name CA)	2.76	0.05	0.05
60	assign (segid 3A4 and resid 97 and name O) (segid 3A4 and resid 98 and name CB)	4.26	0.07	0.07
	assign (segid 3A4 and resid 97 and name O) (segid 3A4 and resid 98 and name N)	2.25	0.02	0.01
	assign (segid 3A4 and resid 97 and name O) (segid 3A4 and resid 98 and name O)	3.35	0.08	0.08
	assign (segid 3A4 and resid 97 and name O) (segid 3A4 and resid 99 and name C)	4.06	0.13	0.13
	assign (segid 3A4 and resid 97 and name O) (segid 3A4 and resid 99 and name CA)	4.35	0.12	0.12
65	assign (segid 3A4 and resid 97 and name O) (segid 3A4 and resid 99 and name CB)	5.30	0.11	0.11
	assign (segid 3A4 and resid 97 and name O) (segid 3A4 and resid 99 and name N)	3.41	0.08	0.08
	assign (segid 3A4 and resid 97 and name O) (segid 3A4 and resid 99 and name O)	4.98	0.13	0.12
	assign (segid 3A4 and resid 98 and name C) (segid 3A4 and resid 100 and name C)	4.58	0.07	0.07
	assign (segid 3A4 and resid 98 and name C) (segid 3A4 and resid 100 and name CA)	4.46	0.05	0.06
	assign (segid 3A4 and resid 98 and name C) (segid 3A4 and resid 100 and name CB)	5.20	0.10	0.11
70	assign (segid 3A4 and resid 98 and name C) (segid 3A4 and resid 100 and name N)	3.28	0.07	0.07
	assign (segid 3A4 and resid 98 and name C) (segid 3A4 and resid 100 and name O)	5.63	0.09	0.09
	assign (segid 3A4 and resid 98 and name C) (segid 3A4 and resid 101 and name C)	4.97	0.09	0.09
	assign (segid 3A4 and resid 98 and name C) (segid 3A4 and resid 101 and name CA)	4.70	0.14	0.14
75	assign (segid 3A4 and resid 98 and name C) (segid 3A4 and resid 101 and name CB)	4.59	0.24	0.24
	assign (segid 3A4 and resid 98 and name C) (segid 3A4 and resid 101 and name CG)	5.90	0.29	0.29
	assign (segid 3A4 and resid 98 and name C) (segid 3A4 and resid 101 and name N)	3.93	0.10	0.09
	assign (segid 3A4 and resid 98 and name C) (segid 3A4 and resid 101 and name O)	6.17	0.09	0.09
	assign (segid 3A4 and resid 98 and name C) (segid 3A4 and resid 102 and name C)	6.11	0.04	0.03
80	assign (segid 3A4 and resid 98 and name C) (segid 3A4 and resid 102 and name CA)	5.02	0.06	0.05
	assign (segid 3A4 and resid 98 and name C) (segid 3A4 and resid 102 and name N)	4.18	0.07	0.06
	assign (segid 3A4 and resid 98 and name C) (segid 3A4 and resid 102 and name O)	7.26	0.04	0.04
	assign (segid 3A4 and resid 98 and name C) (segid 3A4 and resid 103 and name CA)	7.28	0.12	0.11

	assign (segid 3A4 and resid 98 and name C) (segid 3A4 and resid 103 and name CB)	7.30	0.19	0.20
	assign (segid 3A4 and resid 98 and name C) (segid 3A4 and resid 103 and name N)	5.99	0.09	0.09
	assign (segid 3A4 and resid 98 and name C) (segid 3A4 and resid 104 and name N)	7.90	0.07	0.07
	assign (segid 3A4 and resid 98 and name C) (segid 3A4 and resid 403 and name CB)	5.73	0.63	0.63
5	assign (segid 3A4 and resid 98 and name C) (segid 3A4 and resid 98 and name CB)	2.51	0.05	0.05
	assign (segid 3A4 and resid 98 and name C) (segid 3A4 and resid 98 and name O)	1.23	0.01	0.01
	assign (segid 3A4 and resid 98 and name C) (segid 3A4 and resid 99 and name C)	3.03	0.04	0.04
	assign (segid 3A4 and resid 98 and name C) (segid 3A4 and resid 99 and name CA)	2.43	0.01	0.02
	assign (segid 3A4 and resid 98 and name C) (segid 3A4 and resid 99 and name CB)	3.67	0.03	0.04
10	assign (segid 3A4 and resid 98 and name C) (segid 3A4 and resid 99 and name N)	1.32	0.02	0.02
	assign (segid 3A4 and resid 98 and name C) (segid 3A4 and resid 99 and name O)	3.87	0.06	0.06
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 100 and name C)	5.54	0.09	0.10
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 100 and name CA)	5.46	0.06	0.06
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 100 and name CB)	5.87	0.15	0.15
15	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 100 and name O)	4.39	0.06	0.05
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 101 and name C)	6.67	0.12	0.11
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 101 and name CA)	5.83	0.14	0.14
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 101 and name CB)	5.32	0.20	0.20
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 101 and name CG)	4.79	0.31	0.31
20	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 101 and name N)	6.01	0.37	0.36
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 101 and name O)	4.68	0.13	0.13
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 102 and name C)	7.02	0.15	0.14
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 102 and name CA)	7.38	0.06	0.06
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 102 and name N)	6.17	0.06	0.06
25	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 102 and name O)	5.23	0.10	0.09
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 103 and name CB)	8.67	0.12	0.12
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 103 and name N)	8.73	0.19	0.19
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 103 and name O)	7.35	0.10	0.10
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 104 and name CA)	10.04	0.09	0.10
30	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 104 and name CB)	9.65	0.12	0.12
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 105 and name CA)	10.69	0.22	0.21
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 105 and name CB)	9.89	0.24	0.25
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 106 and name CA)	12.34	0.11	0.10
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 106 and name CB)	11.91	0.09	0.10
35	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 107 and name CA)	14.31	0.06	0.07
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 107 and name CB)	13.99	0.04	0.04
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 108 and name CA)	15.57	0.08	0.08
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 108 and name CB)	14.91	0.14	0.14
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 109 and name CA)	16.74	0.28	0.28
40	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 109 and name CB)	16.04	0.33	0.32
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 110 and name CA)	18.37	0.11	0.10
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 110 and name CB)	17.85	0.12	0.13
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 125 and name CA)	14.08	1.23	1.22
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 125 and name CB)	14.39	1.15	1.15
45	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 126 and name CA)	14.15	0.99	1.00
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 127 and name CA)	14.35	1.50	1.51
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 127 and name CB)	15.45	1.78	1.77
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 128 and name CA)	11.75	2.02	2.02
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 128 and name CB)	11.88	2.17	2.18
50	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 129 and name CA)	9.46	1.22	1.22
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 129 and name CB)	9.69	1.16	1.15
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 130 and name CA)	10.40	1.12	1.12
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 130 and name CB)	11.56	1.14	1.13
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 131 and name CA)	11.17	1.58	1.58
55	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 131 and name CB)	11.97	2.02	2.03
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 132 and name CA)	8.83	1.96	1.96
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 132 and name CB)	8.37	2.06	2.06
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 133 and name CA)	8.07	1.07	1.07
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 133 and name CB)	7.93	1.58	1.57
60	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 134 and name CA)	10.75	0.71	0.71
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 135 and name CA)	11.23	1.78	1.78
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 135 and name CB)	11.14	2.39	2.39
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 136 and name CA)	9.79	1.24	1.24
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 136 and name CB)	8.68	1.16	1.15
65	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 137 and name CA)	11.18	0.78	0.78
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 138 and name CA)	14.15	0.62	0.62
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 138 and name CB)	14.77	0.57	0.57
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 139 and name CA)	14.07	1.51	1.50
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 140 and name CA)	15.18	1.64	1.64
70	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 140 and name CB)	15.58	1.26	1.26
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 141 and name CA)	15.22	2.33	2.34
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 219 and name CA)	14.21	1.26	1.27
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 219 and name CB)	14.30	1.37	1.37
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 220 and name CA)	15.39	0.84	0.84
75	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 220 and name CB)	14.83	0.72	0.72
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 221 and name CA)	18.30	0.95	0.96
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 221 and name CB)	18.39	1.02	1.02
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 223 and name CA)	18.42	0.84	0.83
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 251 and name CA)	16.85	0.96	0.96
80	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 251 and name CB)	16.32	1.11	1.11
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 252 and name CA)	16.42	1.07	1.07
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 252 and name CB)	17.23	1.22	1.22
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 254 and name CA)	17.96	0.76	0.76

5	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 255 and name CA)	14.58	0.94	0.93
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 256 and name CA)	14.60	0.75	0.74
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 257 and name CA)	17.37	0.76	0.77
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 258 and name CA)	16.95	0.72	0.71
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 259 and name CB)	17.01	0.76	0.76
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 260 and name CA)	13.55	0.72	0.71
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 261 and name CB)	12.22	0.73	0.74
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 262 and name CA)	14.74	1.02	1.02
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 263 and name CB)	15.36	1.19	1.20
10	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 264 and name CA)	17.95	0.75	0.76
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 265 and name CB)	16.63	0.48	0.48
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 266 and name CA)	15.81	0.41	0.42
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 267 and name CB)	14.78	0.66	0.67
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 268 and name CA)	13.64	0.76	0.76
15	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 269 and name CB)	18.02	0.76	0.77
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 270 and name CA)	18.48	0.60	0.59
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 271 and name CB)	16.47	0.76	0.77
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 272 and name CA)	15.25	0.83	0.83
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 273 and name CB)	16.10	0.71	0.72
20	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 274 and name CA)	18.70	0.57	0.56
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 275 and name CB)	16.52	0.48	0.48
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 276 and name CA)	15.17	0.48	0.47
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 277 and name CB)	19.36	0.50	0.51
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 278 and name CA)	19.10	0.39	0.39
25	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 279 and name CB)	18.32	0.44	0.45
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 280 and name CA)	17.44	0.42	0.43
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 281 and name CB)	17.84	0.41	0.42
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 282 and name CA)	14.01	0.47	0.47
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 283 and name CB)	14.61	0.42	0.41
30	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 284 and name CA)	15.91	0.48	0.47
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 285 and name CB)	12.27	0.64	0.63
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 286 and name CA)	9.32	0.47	0.48
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 287 and name CB)	9.44	0.62	0.62
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 288 and name CA)	10.78	0.49	0.49
35	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 289 and name CB)	12.22	0.49	0.49
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 290 and name CA)	11.35	0.32	0.32
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 291 and name CB)	12.33	0.45	0.45
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 292 and name C)	7.34	0.29	0.30
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 293 and name CA)	8.07	0.47	0.48
40	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 294 and name CB)	7.39	0.65	0.66
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 295 and name O)	7.24	0.28	0.28
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 296 and name CA)	6.87	0.66	0.66
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 297 and name CB)	7.17	0.83	0.82
45	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 298 and name CA)	10.21	0.60	0.60
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 299 and name CB)	10.45	0.31	0.31
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 300 and name CA)	10.60	0.36	0.36
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 301 and name CB)	7.69	0.44	0.43
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 302 and name CA)	6.23	0.16	0.46
50	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 303 and name CB)	9.09	0.89	0.90
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 304 and name CA)	9.34	0.98	0.99
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 305 and name CB)	12.50	0.73	0.74
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 306 and name CA)	13.24	0.69	0.70
	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 307 and name CB)	12.47	0.53	0.53
55	assign (segid 3A4 and resid 98 and name CA) (segid 3A4 and resid 308 and name CA)			

5	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 104 and name CB) 11.27 0.06 0.07
	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 104 and name CB) 10.97 0.08 0.08
	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 105 and name CB) 11.59 0.25 0.25
	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 105 and name CB) 10.68 0.28 0.27
	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 106 and name CB) 13.06 0.13 0.13
	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 106 and name CB) 12.56 0.10 0.10
	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 107 and name CB) 15.31 0.10 0.09
	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 107 and name CB) 15.08 0.07 0.07
10	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 108 and name CB) 16.59 0.13 0.13
	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 108 and name CB) 15.95 0.15 0.15
	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 109 and name CB) 17.50 0.31 0.32
	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 109 and name CB) 16.69 0.36 0.36
	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 110 and name CB) 19.15 0.11 0.11
15	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 110 and name CB) 18.67 0.13 0.13
	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 125 and name CB) 14.53 1.42 1.42
	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 125 and name CB) 14.76 1.33 1.32
	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 126 and name CB) 14.43 1.22 1.22
	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 127 and name CB) 14.86 1.63 1.63
20	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 128 and name CB) 12.43 2.19 2.19
	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 128 and name CB) 12.59 2.40 2.39
	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 129 and name CB) 9.92 1.47 1.47
	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 129 and name CB) 10.02 1.35 1.35
	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 130 and name CB) 10.70 1.49 1.49
	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 130 and name CB) 11.79 1.56 1.55
25	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 131 and name CB) 11.79 1.70 1.71
	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 131 and name CB) 12.67 2.05 2.06
	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 132 and name CB) 9.61 2.15 2.16
	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 132 and name CB) 9.16 2.35 2.35
	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 133 and name CB) 8.54 1.37 1.37
30	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 133 and name CB) 8.23 1.80 1.80
	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 134 and name CB) 11.17 1.14 1.15
	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 135 and name CB) 11.96 1.83 1.83
	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 135 and name CB) 11.99 2.37 2.38
	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 136 and name CB) 10.44 1.49 1.49
35	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 136 and name CB) 9.30 1.47 1.47
	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 137 and name CB) 11.51 1.09 1.10
	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 138 and name CB) 14.62 0.90 0.91
	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 138 and name CB) 15.25 0.88 0.88
	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 139 and name CB) 14.82 1.53 1.53
40	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 140 and name CB) 16.09 1.64 1.64
	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 140 and name CB) 16.44 1.33 1.33
	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 219 and name CB) 14.54 1.31 1.30
	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 219 and name CB) 14.75 1.42 1.42
45	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 220 and name CB) 15.46 0.87 0.87
	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 220 and name CB) 14.84 0.75 0.76
	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 221 and name CB) 18.55 1.00 1.00
	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 223 and name CB) 18.34 0.81 0.81
	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 251 and name CB) 16.65 1.16 1.17
50	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 251 and name CB) 16.15 1.28 1.28
	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 252 and name CB) 16.48 1.30 1.30
	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 254 and name CB) 17.62 1.04 1.04
	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 255 and name CB) 14.28 1.10 1.10
	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 256 and name CB) 14.55 0.96 0.97
	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 257 and name CB) 17.23 1.07 1.06
55	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 258 and name CB) 16.50 1.05 1.04
	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 258 and name CB) 16.48 1.08 1.07
	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 259 and name CB) 13.09 1.06 1.07
	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 259 and name CB) 11.79 1.10 1.11
	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 260 and name CB) 14.60 1.34 1.34
60	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 260 and name CB) 15.33 1.50 1.49
	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 262 and name CB) 16.08 0.78 0.77
	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 262 and name CB) 15.17 0.69 0.68
	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 263 and name CB) 14.41 0.95 0.96
	assign (segid 3A4 and resid 98 and name CB) (segid

	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 392 and name CB)	17.03	0.42	0.41
	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 393 and name CA)	13.13	0.58	0.58
	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 394 and name CA)	13.49	0.39	0.39
	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 394 and name CB)	14.74	0.36	0.36
5	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 395 and name CA)	11.04	0.36	0.35
	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 396 and name CA)	8.29	0.54	0.54
	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 396 and name CB)	8.57	0.72	0.71
	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 397 and name CA)	9.80	0.82	0.82
	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 397 and name CB)	11.27	0.81	0.80
10	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 398 and name CA)	10.14	0.44	0.44
	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 398 and name CB)	11.05	0.38	0.38
	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 399 and name C)	6.18	0.60	0.61
	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 399 and name CA)	6.81	0.46	0.45
	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 399 and name CB)	6.11	0.55	0.55
15	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 399 and name O)	6.15	0.59	0.58
	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 400 and name CA)	6.00	1.14	1.13
	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 400 and name CB)	6.43	1.31	1.31
	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 401 and name CA)	9.38	0.96	0.96
	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 402 and name CA)	9.47	0.50	0.50
20	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 402 and name CB)	9.50	0.38	0.37
	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 403 and name CA)	7.03	0.63	0.63
	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 403 and name CB)	5.59	0.70	0.69
	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 404 and name CA)	8.85	1.12	1.11
	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 404 and name CB)	9.10	1.23	1.24
25	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 405 and name CA)	12.05	0.92	0.93
	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 405 and name CB)	12.66	0.90	0.90
	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 406 and name CA)	12.01	0.59	0.58
	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 407 and name CA)	11.55	0.73	0.74
	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 407 and name CB)	10.41	0.81	0.81
30	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 408 and name CA)	13.95	0.96	0.96
	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 408 and name CB)	14.04	1.02	1.02
	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 409 and name CA)	16.62	0.77	0.76
	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 409 and name CB)	16.84	0.80	0.80
	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 410 and name CA)	16.65	0.61	0.62
35	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 411 and name CA)	17.30	0.66	0.66
	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 411 and name CB)	16.36	0.74	0.73
	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 99 and name C)	5.45	0.04	0.04
	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 99 and name CA)	4.49	0.04	0.04
	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 99 and name CB)	5.31	0.09	0.09
40	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 99 and name N)	3.17	0.05	0.04
	assign (segid 3A4 and resid 98 and name CB) (segid 3A4 and resid 99 and name O)	6.32	0.05	0.04
	assign (segid 3A4 and resid 98 and name N) (segid 3A4 and resid 100 and name C)	5.69	0.12	0.11
	assign (segid 3A4 and resid 98 and name N) (segid 3A4 and resid 100 and name CA)	5.33	0.08	0.07
	assign (segid 3A4 and resid 98 and name N) (segid 3A4 and resid 100 and name CB)	5.39	0.14	0.14
45	assign (segid 3A4 and resid 98 and name N) (segid 3A4 and resid 100 and name N)	4.31	0.06	0.06
	assign (segid 3A4 and resid 98 and name N) (segid 3A4 and resid 100 and name O)	6.90	0.12	0.11
	assign (segid 3A4 and resid 98 and name N) (segid 3A4 and resid 101 and name C)	6.59	0.15	0.15
	assign (segid 3A4 and resid 98 and name N) (segid 3A4 and resid 101 and name CA)	5.81	0.23	0.23
	assign (segid 3A4 and resid 98 and name N) (segid 3A4 and resid 101 and name CB)	5.35	0.34	0.34
50	assign (segid 3A4 and resid 98 and name N) (segid 3A4 and resid 101 and name CG)	6.67	0.38	0.38
	assign (segid 3A4 and resid 98 and name N) (segid 3A4 and resid 101 and name N)	4.95	0.16	0.17
	assign (segid 3A4 and resid 98 and name N) (segid 3A4 and resid 102 and name CA)	7.22	0.06	0.06
	assign (segid 3A4 and resid 98 and name N) (segid 3A4 and resid 102 and name N)	6.15	0.10	0.09
	assign (segid 3A4 and resid 98 and name N) (segid 3A4 and resid 98 and name C)	2.44	0.04	0.03
55	assign (segid 3A4 and resid 98 and name N) (segid 3A4 and resid 98 and name CA)	1.46	0.01	0.00
	assign (segid 3A4 and resid 98 and name N) (segid 3A4 and resid 98 and name CB)	2.47	0.02	0.03
	assign (segid 3A4 and resid 98 and name N) (segid 3A4 and resid 98 and name O)	3.45	0.02	0.02
	assign (segid 3A4 and resid 98 and name N) (segid 3A4 and resid 99 and name C)	4.71	0.05	0.05
	assign (segid 3A4 and resid 98 and name N) (segid 3A4 and resid 99 and name CA)	4.22	0.08	0.08
60	assign (segid 3A4 and resid 98 and name N) (segid 3A4 and resid 99 and name CB)	4.94	0.09	0.09
	assign (segid 3A4 and resid 98 and name N) (segid 3A4 and resid 99 and name N)	2.81	0.09	0.09
	assign (segid 3A4 and resid 98 and name N) (segid 3A4 and resid 99 and name O)	5.79	0.06	0.06
	assign (segid 3A4 and resid 98 and name O) (segid 3A4 and resid 100 and name C)	4.08	0.10	0.09
	assign (segid 3A4 and resid 98 and name O) (segid 3A4 and resid 100 and name CA)	4.33	0.10	0.11
65	assign (segid 3A4 and resid 98 and name O) (segid 3A4 and resid 100 and name CB)	5.28	0.12	0.11
	assign (segid 3A4 and resid 98 and name O) (segid 3A4 and resid 100 and name N)	3.39	0.10	0.10
	assign (segid 3A4 and resid 98 and name O) (segid 3A4 and resid 100 and name O)	4.98	0.12	0.12
	assign (segid 3A4 and resid 98 and name O) (segid 3A4 and resid 101 and name C)	3.88	0.08	0.09
	assign (segid 3A4 and resid 98 and name O) (segid 3A4 and resid 101 and name CA)	3.85	0.12	0.13
70	assign (segid 3A4 and resid 98 and name O) (segid 3A4 and resid 101 and name CB)	3.83	0.20	0.20
	assign (segid 3A4 and resid 98 and name O) (segid 3A4 and resid 101 and name CG)	5.04	0.27	0.26
	assign (segid 3A4 and resid 98 and name O) (segid 3A4 and resid 101 and name N)	3.33	0.09	0.10
	assign (segid 3A4 and resid 98 and name O) (segid 3A4 and resid 101 and name O)	5.05	0.08	0.09
	assign (segid 3A4 and resid 98 and name O) (segid 3A4 and resid 102 and name C)	5.02	0.06	0.06
75	assign (segid 3A4 and resid 98 and name O) (segid 3A4 and resid 102 and name CA)	3.84	0.06	0.06
	assign (segid 3A4 and resid 98 and name O) (segid 3A4 and resid 102 and name N)	3.01	0.07	0.07
	assign (segid 3A4 and resid 98 and name O) (segid 3A4 and resid 102 and name O)	6.14	0.06	0.05
	assign (segid 3A4 and resid 98 and name O) (segid 3A4 and resid 103 and name C)	7.27	0.09	0.10
80	assign (segid 3A4 and resid 98 and name O) (segid 3A4 and resid 103 and name CA)	6.42	0.13	0.12
	assign (segid 3A4 and resid 98 and name O) (segid 3A4 and resid 103 and name CB)	6.65	0.19	0.19
	assign (segid 3A4 and resid 98 and name O) (segid 3A4 and resid 103 and name N)	5.05	0.12	0.11
	assign (segid 3A4 and resid 98 and name O) (segid 3A4 and resid 104 and name N)	6.97	0.09	0.09
	assign (segid 3A4 and resid 98 and name O) (segid 3A4 and resid 403 and name CA)	6.85	0.46	0.45

	assign	(segid 3A4 and resid 98 and name O)	(segid 3A4 and resid 98 and name CB)	5.55	0.44	0.44
	assign	(segid 3A4 and resid 98 and name O)	(segid 3A4 and resid 99 and name CB)	3.30	0.10	0.10
	assign	(segid 3A4 and resid 98 and name O)	(segid 3A4 and resid 99 and name CA)	2.96	0.07	0.07
	assign	(segid 3A4 and resid 98 and name O)	(segid 3A4 and resid 99 and name CB)	2.76	0.05	0.04
5	assign	(segid 3A4 and resid 98 and name O)	(segid 3A4 and resid 99 and name N)	4.22	0.04	0.04
	assign	(segid 3A4 and resid 98 and name O)	(segid 3A4 and resid 99 and name O)	2.24	0.02	0.01
	assign	(segid 3A4 and resid 99 and name C)	(segid 3A4 and resid 100 and name O)	3.44	0.09	0.10
	assign	(segid 3A4 and resid 99 and name C)	(segid 3A4 and resid 100 and name CA)	3.02	0.03	0.02
	assign	(segid 3A4 and resid 99 and name C)	(segid 3A4 and resid 100 and name CB)	2.44	0.03	0.02
10	assign	(segid 3A4 and resid 99 and name C)	(segid 3A4 and resid 100 and name N)	3.73	0.02	0.01
	assign	(segid 3A4 and resid 99 and name C)	(segid 3A4 and resid 100 and name O)	1.34	0.01	0.01
	assign	(segid 3A4 and resid 99 and name C)	(segid 3A4 and resid 101 and name O)	3.79	0.06	0.07
	assign	(segid 3A4 and resid 99 and name C)	(segid 3A4 and resid 101 and name CA)	4.57	0.06	0.05
	assign	(segid 3A4 and resid 99 and name C)	(segid 3A4 and resid 101 and name CB)	4.53	0.05	0.05
15	assign	(segid 3A4 and resid 99 and name C)	(segid 3A4 and resid 101 and name CG)	5.35	0.10	0.10
	assign	(segid 3A4 and resid 99 and name C)	(segid 3A4 and resid 101 and name N)	6.71	0.12	0.13
	assign	(segid 3A4 and resid 99 and name C)	(segid 3A4 and resid 101 and name O)	3.36	0.05	0.05
	assign	(segid 3A4 and resid 99 and name C)	(segid 3A4 and resid 101 and name O)	5.62	0.07	0.07
	assign	(segid 3A4 and resid 99 and name C)	(segid 3A4 and resid 102 and name C)	4.85	0.08	0.08
20	assign	(segid 3A4 and resid 99 and name C)	(segid 3A4 and resid 102 and name CA)	4.52	0.08	0.08
	assign	(segid 3A4 and resid 99 and name C)	(segid 3A4 and resid 102 and name N)	3.83	0.06	0.07
	assign	(segid 3A4 and resid 99 and name C)	(segid 3A4 and resid 102 and name O)	6.06	0.09	0.08
	assign	(segid 3A4 and resid 99 and name C)	(segid 3A4 and resid 102 and name O)	6.13	0.14	0.13
	assign	(segid 3A4 and resid 99 and name C)	(segid 3A4 and resid 103 and name CA)	5.04	0.14	0.14
25	assign	(segid 3A4 and resid 99 and name C)	(segid 3A4 and resid 103 and name CB)	4.64	0.22	0.21
	assign	(segid 3A4 and resid 99 and name C)	(segid 3A4 and resid 103 and name N)	4.13	0.10	0.10
	assign	(segid 3A4 and resid 99 and name C)	(segid 3A4 and resid 103 and name O)	7.28	0.13	0.14
	assign	(segid 3A4 and resid 99 and name C)	(segid 3A4 and resid 103 and name O)	7.30	0.12	0.11
	assign	(segid 3A4 and resid 99 and name C)	(segid 3A4 and resid 104 and name CA)	7.34	0.13	0.14
	assign	(segid 3A4 and resid 99 and name C)	(segid 3A4 and resid 104 and name CB)	6.02	0.12	0.12
30	assign	(segid 3A4 and resid 99 and name C)	(segid 3A4 and resid 104 and name N)	7.85	0.04	0.04
	assign	(segid 3A4 and resid 99 and name C)	(segid 3A4 and resid 105 and name N)	2.52	0.02	0.03
	assign	(segid 3A4 and resid 99 and name C)	(segid 3A4 and resid 99 and name CB)	1.23	0.00	0.01
	assign	(segid 3A4 and resid 99 and name CA)	(segid 3A4 and resid 100 and name C)	4.41	0.04	0.04
35	assign	(segid 3A4 and resid 99 and name CA)	(segid 3A4 and resid 100 and name CA)	3.82	0.03	0.03
	assign	(segid 3A4 and resid 99 and name CA)	(segid 3A4 and resid 100 and name CB)	4.90	0.02	0.02
	assign	(segid 3A4 and resid 99 and name CA)	(segid 3A4 and resid 100 and name N)	2.45	0.02	0.03
	assign	(segid 3A4 and resid 99 and name CA)	(segid 3A4 and resid 100 and name O)	5.25	0.07	0.08
	assign	(segid 3A4 and resid 99 and name CA)	(segid 3A4 and resid 101 and name C)	5.51	0.07	0.08
40	assign	(segid 3A4 and resid 99 and name CA)	(segid 3A4 and resid 101 and name CA)	5.54	0.08	0.07
	assign	(segid 3A4 and resid 99 and name CA)	(segid 3A4 and resid 101 and name CB)	6.05	0.16	0.15
	assign	(segid 3A4 and resid 99 and name CA)	(segid 3A4 and resid 101 and name CG)	7.39	0.20	0.20
	assign	(segid 3A4 and resid 99 and name CA)	(segid 3A4 and resid 101 and name N)	4.46	0.05	0.06
	assign	(segid 3A4 and resid 99 and name CA)	(segid 3A4 and resid 101 and name O)	6.61	0.09	0.09
45	assign	(segid 3A4 and resid 99 and name CA)	(segid 3A4 and resid 102 and name C)	5.64	0.11	0.11
	assign	(segid 3A4 and resid 99 and name CA)	(segid 3A4 and resid 102 and name CA)	5.06	0.11	0.11
	assign	(segid 3A4 and resid 99 and name CA)	(segid 3A4 and resid 102 and name N)	4.55	0.08	0.09
	assign	(segid 3A4 and resid 99 and name CA)	(segid 3A4 and resid 102 and name O)	6.82	0.13	0.13
	assign	(segid 3A4 and resid 99 and name CA)	(segid 3			

assign (segid 3A4 and resid 99 and name CA) (segid 3A4 and resid 133 and name CA) 11.18 0.86 0.85
assign (segid 3A4 and resid 99 and name CA) (segid 3A4 and resid 133 and name CB) 11.11 1.57 1.56
assign (segid 3A4 and resid 99 and name CA) (segid 3A4 and resid 134 and name CA) 13.87 0.21 0.21
assign (segid 3A4 and resid 99 and name CA) (segid 3A4 and resid 135 and name CA) 14.00 1.66 1.65
5 assign (segid 3A4 and resid 99 and name CA) (segid 3A4 and resid 135 and name CB) 13.70 2.29 2.29
assign (segid 3A4 and resid 99 and name CA) (segid 3A4 and resid 136 and name CA) 12.66 0.83 0.83
assign (segid 3A4 and resid 99 and name CA) (segid 3A4 and resid 136 and name CB) 11.55 0.65 0.66
assign (segid 3A4 and resid 99 and name CA) (segid 3A4 and resid 137 and name CA) 14.39 0.73 0.72
assign (segid 3A4 and resid 99 and name CA) (segid 3A4 and resid 138 and name CA) 17.18 0.56 0.56
10 assign (segid 3A4 and resid 99 and name CA) (segid 3A4 and resid 138 and name CB) 17.82 0.50 0.50
assign (segid 3A4 and resid 99 and name CA) (segid 3A4 and resid 139 and name CA) 16.60 1.58 1.58
assign (segid 3A4 and resid 99 and name CA) (segid 3A4 and resid 219 and name CA) 17.00 1.40 1.41
assign (segid 3A4 and resid 99 and name CA) (segid 3A4 and resid 219 and name CB) 17.07 1.46 1.46
assign (segid 3A4 and resid 99 and name CA) (segid 3A4 and resid 220 and name CB) 18.17 0.91 0.92
15 assign (segid 3A4 and resid 99 and name CA) (segid 3A4 and resid 255 and name CA) 17.82 0.72 0.72
assign (segid 3A4 and resid 99 and name CA) (segid 3A4 and resid 256 and name CA) 17.52 0.60 0.59
assign (segid 3A4 and resid 99 and name CA) (segid 3A4 and resid 259 and name CA) 15.97 0.69 0.68
assign (segid 3A4 and resid 99 and name CA) (segid 3A4 and resid 259 and name CB) 14.78 0.65 0.66
20 assign (segid 3A4 and resid 99 and name CA) (segid 3A4 and resid 260 and name CA) 16.71 0.98 0.97
assign (segid 3A4 and resid 99 and name CA) (segid 3A4 and resid 262 and name CB) 17.66 0.57 0.56
assign (segid 3A4 and resid 99 and name CA) (segid 3A4 and resid 263 and name CA) 15.89 0.91 0.91
assign (segid 3A4 and resid 99 and name CA) (segid 3A4 and resid 263 and name CB) 14.76 0.94 0.93
assign (segid 3A4 and resid 99 and name CA) (segid 3A4 and resid 305 and name CA) 16.07 1.32 1.32
assign (segid 3A4 and resid 99 and name CA) (segid 3A4 and resid 305 and name CB) 14.67 1.38 1.38
25 assign (segid 3A4 and resid 99 and name CA) (segid 3A4 and resid 306 and name CA) 16.42 0.95 0.95
assign (segid 3A4 and resid 99 and name CA) (segid 3A4 and resid 309 and name CA) 17.35 1.07 1.07
assign (segid 3A4 and resid 99 and name CA) (segid 3A4 and resid 309 and name CB) 16.05 1.02 1.02
assign (segid 3A4 and resid 99 and name CA) (segid 3A4 and resid 393 and name CA) 17.34 0.37 0.37
30 assign (segid 3A4 and resid 99 and name CA) (segid 3A4 and resid 394 and name CA) 17.51 0.33 0.32
assign (segid 3A4 and resid 99 and name CA) (segid 3A4 and resid 394 and name CB) 18.72 0.33 0.33
assign (segid 3A4 and resid 99 and name CA) (segid 3A4 and resid 395 and name CA) 14.96 0.32 0.33
assign (segid 3A4 and resid 99 and name CA) (segid 3A4 and resid 396 and name CA) 12.39 0.39 0.39
assign (segid 3A4 and resid 99 and name CA) (segid 3A4 and resid 396 and name CB) 12.73 0.55 0.56
35 assign (segid 3A4 and resid 99 and name CA) (segid 3A4 and resid 397 and name CA) 13.54 0.56 0.55
assign (segid 3A4 and resid 99 and name CA) (segid 3A4 and resid 397 and name CB) 14.99 0.56 0.57
assign (segid 3A4 and resid 99 and name CA) (segid 3A4 and resid 398 and name CA) 13.37 0.50 0.51
assign (segid 3A4 and resid 99 and name CA) (segid 3A4 and resid 398 and name CB) 14.29 0.45 0.46
40 assign (segid 3A4 and resid 99 and name CA) (segid 3A4 and resid 399 and name CA) 9.90 0.50 0.50
assign (segid 3A4 and resid 99 and name CA) (segid 3A4 and resid 399 and name CB) 9.49 0.51 0.52
assign (segid 3A4 and resid 99 and name CA) (segid 3A4 and resid 400 and name CA) 8.85 0.88 0.89
assign (segid 3A4 and resid 99 and name CA) (segid 3A4 and resid 400 and name CB) 9.56 0.91 0.91
45 assign (segid 3A4 and resid 99 and name CA) (segid 3A4 and resid 401 and name CA) 11.43 1.07 1.07
assign (segid 3A4 and resid 99 and name CA) (segid 3A4 and resid 402 and name CA) 10.77 0.94 0.94
assign (segid 3A4 and resid 99 and name CA) (segid 3A4 and resid 402 and name CB) 11.02 0.80 0.79
50 assign (segid 3A4 and resid 99 and name CA) (segid 3A4 and resid 403 and name CA) 7.25 1.10 1.09
assign (segid 3A4 and resid 99 and name CA) (segid 3A4 and resid 403 and name CB) 6.04 1.04 1.05
assign (segid 3A4 and resid 99 and name CA) (segid 3A4 and resid 404 and name CA) 8.73 1.36 1.37
assign (segid 3A4 and resid 99 and name CA) (segid 3A4 and resid 404 and name CB) 9.49 1.31 1.32
55 assign (segid 3A4 and resid 99 and name CA) (segid 3A4 and resid 405 and name CA) 11.89 1.38 1.38
assign (segid 3A4 and resid 99 and name CA) (segid 3A4 and resid 405 and name CB) 12.90 1.33 1.32
assign (segid 3A4 and resid 99 and name CA) (segid 3A4 and resid 406 and name CA) 11.00 1.36 1.37
assign (segid 3A4 and resid 99 and name CA) (segid 3A4 and resid 407 and name CA) 9.45 1.45 1.45
assign (segid 3A4 and resid 99 and name CA) (segid 3A4 and resid 407 and name CB) 8.11 1.49 1.50
60 assign (segid 3A4 and resid 99 and name CA) (segid 3A4 and resid 408 and name CA) 12.27 1.52 1.51
assign (segid 3A4 and resid 99 and name CA) (segid 3A4 and resid 408 and name CB) 12.78 1.53 1.53
assign (segid 3A4 and resid 99 and name CA) (segid 3A4 and resid 409 and name CA) 15.01 1.40 1.40
assign (segid 3A4 and resid 99 and name CA) (segid 3A4 and resid 409 and name CB) 15.52 1.40 1.39
assign (segid 3A4 and resid 99 and name CA) (segid 3A4 and resid 410 and name CA) 14.28 1.23 1.22
assign (segid 3A4 and resid 99 and name CA) (segid 3A4 and resid 411 and name CA) 14.54 1.23 1.22
65 assign (segid 3A4 and resid 99 and name CA) (segid 3A4 and resid 411 and name CB) 13.53 1.26 1.25
assign (segid 3A4 and resid 99 and name CA) (segid 3A4 and resid 99 and name C) 1.53 0.02 0.01
assign (segid 3A4 and resid 99 and name CA) (segid 3A4 and resid 99 and name CB) 1.52 0.01 0.01
assign (segid 3A4 and resid 99 and name CA) (segid 3A4 and resid 99 and name O) 2.40 0.02 0.01
70 assign (segid 3A4 and resid 99 and name CB) (segid 3A4 and resid 100 and name C) 5.46 0.04 0.04
assign (segid 3A4 and resid 99 and name CB) (segid 3A4 and resid 100 and name CA) 4.53 0.05 0.06
assign (segid 3A4 and resid 99 and name CB) (segid 3A4 and resid 100 and name CB) 5.44 0.07 0.06
assign (segid 3A4 and resid 99 and name CB) (segid 3A4 and resid 100 and name N) 3.21 0.06 0.05
assign (segid 3A4 and resid 99 and name CB) (segid 3A4 and resid 100 and name O) 6.26 0.06 0.06
75 assign (segid 3A4 and resid 99 and name CB) (segid 3A4 and resid 101 and name C) 6.92 0.07 0.08
assign (segid 3A4 and resid 99 and name CB) (segid 3A4 and resid 101 and name CA) 6.91 0.06 0.06
assign (segid 3A4 and resid 99 and name CB) (segid 3A4 and resid 101 and name CB) 7.47 0.14 0.15
assign (segid 3A4 and resid 99 and name CB) (segid 3A4 and resid 101 and name N) 5.72 0.05 0.05
assign (segid 3A4 and resid 99 and name CB) (segid 3A4 and resid 102 and name C) 6.80 0.15 0.15
80 assign (segid 3A4 and resid 99 and name CB) (segid 3A4 and resid 102 and name CA) 6.40 0.13 0.13
assign (segid 3A4 and resid 99 and name CB) (segid 3A4 and resid 102 and name N) 5.99 0.09 0.10
assign (segid 3A4 and resid 99 and name CB) (segid 3A4 and resid 103 and name CA) 6.93 0.18 0.19
assign (segid 3A4 and resid 99 and name CB) (segid 3A4 and resid 103 and name CB) 6.36 0.26 0.27
assign (segid 3A4 and resid 99 and name CB) (segid 3A4 and resid 103 and name N) 6.16 0.14 0.13
assign (segid 3A4 and resid 99 and name CB) (segid 3A4 and resid 104 and name CA) 9.68 0.13 0.13
assign (segid 3A4 and resid 99 and name CB) (segid 3A4 and resid 104 and name CB) 9.81 0.14 0.15
assign (segid 3A4 and resid 99 and name CB) (segid 3A4 and resid 105 and name CA) 11.16 0.10 0.11
assign (segid 3A4 and resid 99 and name CB) (segid 3A4 and resid 105 and name CB) 10.81 0.16 0.15
assign (segid 3A4 and resid 99 and name CB) (segid 3A4 and resid 106 and name CA) 11.49 0.21 0.21

	assign	(segid 3A4 and resid 99 and name CB)	(segid 3A4 and resid 106 and name CB)	10.59	0.26	0.25
	assign	(segid 3A4 and resid 99 and name CB)	(segid 3A4 and resid 107 and name CA)	13.02	0.26	0.25
	assign	(segid 3A4 and resid 99 and name CB)	(segid 3A4 and resid 107 and name CB)	12.56	0.26	0.27
	assign	(segid 3A4 and resid 99 and name CB)	(segid 3A4 and resid 108 and name CA)	15.34	0.20	0.20
5	assign	(segid 3A4 and resid 99 and name CB)	(segid 3A4 and resid 108 and name CB)	15.12	0.20	0.20
	assign	(segid 3A4 and resid 99 and name CB)	(segid 3A4 and resid 109 and name CA)	16.50	0.14	0.13
	assign	(segid 3A4 and resid 99 and name CB)	(segid 3A4 and resid 109 and name CB)	15.86	0.19	0.20
	assign	(segid 3A4 and resid 99 and name CB)	(segid 3A4 and resid 110 and name CA)	17.13	0.29	0.28
	assign	(segid 3A4 and resid 99 and name CB)	(segid 3A4 and resid 110 and name CB)	16.27	0.36	0.36
10	assign	(segid 3A4 and resid 99 and name CB)	(segid 3A4 and resid 125 and name CA)	16.07	1.09	1.09
	assign	(segid 3A4 and resid 99 and name CB)	(segid 3A4 and resid 125 and name CB)	16.15	1.24	1.24
	assign	(segid 3A4 and resid 99 and name CB)	(segid 3A4 and resid 126 and name CA)	16.88	1.09	1.08
	assign	(segid 3A4 and resid 99 and name CB)	(segid 3A4 and resid 128 and name CA)	14.65	1.69	1.68
	assign	(segid 3A4 and resid 99 and name CB)	(segid 3A4 and resid 128 and name CB)	14.45	1.83	1.83
15	assign	(segid 3A4 and resid 99 and name CB)	(segid 3A4 and resid 129 and name CA)	12.76	0.91	0.90
	assign	(segid 3A4 and resid 99 and name CB)	(segid 3A4 and resid 129 and name CB)	12.79	1.28	1.28
	assign	(segid 3A4 and resid 99 and name CB)	(segid 3A4 and resid 130 and name CA)	14.30	0.96	0.96
	assign	(segid 3A4 and resid 99 and name CB)	(segid 3A4 and resid 130 and name CB)	15.37	1.05	1.05
20	assign	(segid 3A4 and resid 99 and name CB)	(segid 3A4 and resid 131 and name CA)	14.95	1.31	1.30
	assign	(segid 3A4 and resid 99 and name CB)	(segid 3A4 and resid 131 and name CB)	15.49	1.92	1.93
	assign	(segid 3A4 and resid 99 and name CB)	(segid 3A4 and resid 132 and name CA)	12.63	1.32	1.33
	assign	(segid 3A4 and resid 99 and name CB)	(segid 3A4 and resid 132 and name CB)	12.01	1.25	1.25
	assign	(segid 3A4 and resid 99 and name CB)	(segid 3A4 and resid 133 and name CA)	12.35	0.81	0.80
	assign	(segid 3A4 and resid 99 and name CB)	(segid 3A4 and resid 133 and name CB)	12.30	1.54	1.54
25	assign	(segid 3A4 and resid 99 and name CB)	(segid 3A4 and resid 134 and name CA)	11.96	0.18	0.18
	assign	(segid 3A4 and resid 99 and name CB)	(segid 3A4 and resid 135 and name CA)	15.00	1.75	1.75
	assign	(segid 3A4 and resid 99 and name CB)	(segid 3A4 and resid 135 and name CB)	14.74	2.39	2.39
	assign	(segid 3A4 and resid 99 and name CB)	(segid 3A4 and resid 136 and name CA)	13.46	0.91	0.91
	assign	(segid 3A4 and resid 99 and name CB)	(segid 3A4 and resid 136 and name CB)	12.36	0.69	0.69
30	assign	(segid 3A4 and resid 99 and name CB)	(segid 3A4 and resid 137 and name CA)	15.12	0.73	0.74
	assign	(segid 3A4 and resid 99 and name CB)	(segid 3A4 and resid 138 and name CA)	17.94	0.65	0.65
	assign	(segid 3A4 and resid 99 and name CB)	(segid 3A4 and resid 138 and name CB)	18.66	0.59	0.59
	assign	(segid 3A4 and resid 99 and name CB)	(segid 3A4 and resid 139 and name CA)	17.76	1.68	1.68
	assign	(segid 3A4 and resid 99 and name CB)	(segid 3A4 and resid 256 and name CA)	18.83	0.55	0.56
35	assign	(segid 3A4 and resid 99 and name CB)	(segid 3A4 and resid 259 and name CA)	17.20	0.76	0.76
	assign	(segid 3A4 and resid 99 and name CB)	(segid 3A4 and resid 259 and name CB)	16.02	0.74	0.73
	assign	(segid 3A4 and resid 99 and name CB)	(segid 3A4 and resid 263 and name CA)	17.09	1.03	1.04
	assign	(segid 3A4 and resid 99 and name CB)	(segid 3A4 and resid 263 and name CB)	16.00	1.04	1.05
40	assign	(segid 3A4 and resid 99 and name CB)	(segid 3A4 and resid 305 and name CA)	16.29	1.65	1.65
	assign	(segid 3A4 and resid 99 and name CB)	(segid 3A4 and resid 305 and name CB)	14.87	1.71	1.71
	assign	(segid 3A4 and resid 99 and name CB)	(segid 3A4 and resid 306 and name CA)	16.64	1.26	1.25
	assign	(segid 3A4 and resid 99 and name CB)	(segid 3A4 and resid 309 and name CB)	16.64	1.31	1.31
	assign	(segid 3A4 and resid 99 and name CB)	(segid 3A4 and resid 393 and name CA)	18.07	0.42	0.41
	assign	(segid 3A4 and resid 99 and name CB)	(segid 3A4 and resid 394 and name CA)	18.14	0.45	0.46
45	assign	(segid 3A4 and resid 99 and name CB)	(segid 3A4 and resid 395 and name CA)	15.38	0.38	0.38
	assign	(segid 3A4 and resid 99 and name CB)	(segid 3A4 and resid 396 and name CA)	13.04	0.48	0.49
	assign	(segid 3A4 and resid 99 and name CB)	(segid 3A4 and resid 396 and name CB)	13.44	0.62	0.61
	assign	(segid 3A4 and resid 99 and name CB)	(segid 3A4 and resid 397 and name CA)	14.41	0.72	0.71
	assign	(segid 3A4 and resid 99 and name CB)	(segid 3A4 and resid 397 and name CB)	15.88	0.70	0.71

	assign (segid 3A4 and resid 99 and name N) (segid 3A4 and resid 101 and name O)	6.89	0.06	0.06
	assign (segid 3A4 and resid 99 and name N) (segid 3A4 and resid 102 and name C)	6.43	0.06	0.07
	assign (segid 3A4 and resid 99 and name N) (segid 3A4 and resid 102 and name CA)	5.57	0.08	0.08
	assign (segid 3A4 and resid 99 and name N) (segid 3A4 and resid 102 and name N)	4.84	0.05	0.06
5	assign (segid 3A4 and resid 99 and name N) (segid 3A4 and resid 102 and name O)	7.62	0.07	0.08
	assign (segid 3A4 and resid 99 and name N) (segid 3A4 and resid 103 and name CA)	7.24	0.12	0.12
	assign (segid 3A4 and resid 99 and name N) (segid 3A4 and resid 103 and name CB)	7.03	0.21	0.21
	assign (segid 3A4 and resid 99 and name N) (segid 3A4 and resid 103 and name N)	6.10	0.08	0.08
	assign (segid 3A4 and resid 99 and name N) (segid 3A4 and resid 99 and name C)	2.47	0.02	0.02
10	assign (segid 3A4 and resid 99 and name N) (segid 3A4 and resid 99 and name CA)	1.47	0.01	0.01
	assign (segid 3A4 and resid 99 and name N) (segid 3A4 and resid 99 and name CB)	2.42	0.03	0.03
	assign (segid 3A4 and resid 99 and name N) (segid 3A4 and resid 99 and name O)	3.51	0.03	0.04
	assign (segid 3A4 and resid 99 and name O) (segid 3A4 and resid 100 and name C)	2.93	0.04	0.04
	assign (segid 3A4 and resid 99 and name O) (segid 3A4 and resid 100 and name CA)	2.75	0.03	0.03
15	assign (segid 3A4 and resid 99 and name O) (segid 3A4 and resid 100 and name CB)	4.24	0.02	0.02
	assign (segid 3A4 and resid 99 and name O) (segid 3A4 and resid 100 and name N)	2.25	0.02	0.01
	assign (segid 3A4 and resid 99 and name O) (segid 3A4 and resid 100 and name O)	3.33	0.08	0.07
	assign (segid 3A4 and resid 99 and name O) (segid 3A4 and resid 101 and name C)	4.10	0.09	0.10
	assign (segid 3A4 and resid 99 and name O) (segid 3A4 and resid 101 and name CA)	4.40	0.09	0.10
20	assign (segid 3A4 and resid 99 and name O) (segid 3A4 and resid 101 and name CB)	5.45	0.10	0.09
	assign (segid 3A4 and resid 99 and name O) (segid 3A4 and resid 101 and name CG)	6.65	0.13	0.13
	assign (segid 3A4 and resid 99 and name O) (segid 3A4 and resid 101 and name N)	3.47	0.10	0.10
	assign (segid 3A4 and resid 99 and name O) (segid 3A4 and resid 101 and name O)	4.99	0.11	0.10
	assign (segid 3A4 and resid 99 and name O) (segid 3A4 and resid 102 and name C)	3.80	0.09	0.10
25	assign (segid 3A4 and resid 99 and name O) (segid 3A4 and resid 102 and name CA)	3.76	0.08	0.08
	assign (segid 3A4 and resid 99 and name O) (segid 3A4 and resid 102 and name N)	3.32	0.09	0.10
	assign (segid 3A4 and resid 99 and name O) (segid 3A4 and resid 102 and name O)	4.98	0.09	0.09
	assign (segid 3A4 and resid 99 and name O) (segid 3A4 and resid 103 and name C)	5.01	0.16	0.16
	assign (segid 3A4 and resid 99 and name O) (segid 3A4 and resid 103 and name CA)	3.85	0.15	0.15
30	assign (segid 3A4 and resid 99 and name O) (segid 3A4 and resid 103 and name CB)	3.55	0.21	0.20
	assign (segid 3A4 and resid 99 and name O) (segid 3A4 and resid 103 and name N)	2.98	0.12	0.12
	assign (segid 3A4 and resid 99 and name O) (segid 3A4 and resid 103 and name O)	6.14	0.16	0.16
	assign (segid 3A4 and resid 99 and name O) (segid 3A4 and resid 104 and name C)	7.24	0.11	0.12
	assign (segid 3A4 and resid 99 and name O) (segid 3A4 and resid 104 and name CA)	6.41	0.16	0.15
35	assign (segid 3A4 and resid 99 and name O) (segid 3A4 and resid 104 and name CB)	6.65	0.17	0.17
	assign (segid 3A4 and resid 99 and name O) (segid 3A4 and resid 104 and name N)	5.05	0.16	0.16
	assign (segid 3A4 and resid 99 and name O) (segid 3A4 and resid 105 and name CB)	7.83	0.07	0.07
	assign (segid 3A4 and resid 99 and name O) (segid 3A4 and resid 105 and name N)	6.92	0.05	0.05
	assign (segid 3A4 and resid 99 and name O) (segid 3A4 and resid 106 and name N)	7.76	0.09	0.09
40	assign (segid 3A4 and resid 99 and name O) (segid 3A4 and resid 99 and name CB)	3.32	0.06	0.07
	assign (segid 3A4 and resid 99 and name C) (segid 3A4 and resid 10 and name C)	3.04	0.06	0.06
	assign (segid 3A4 and resid 99 and name C) (segid 3A4 and resid 10 and name CA)	2.44	0.02	0.02
	assign (segid 3A4 and resid 99 and name C) (segid 3A4 and resid 10 and name CB)	3.73	0.02	0.01
	assign (segid 3A4 and resid 99 and name C) (segid 3A4 and resid 10 and name N)	1.33	0.02	0.01
45	assign (segid 3A4 and resid 99 and name C) (segid 3A4 and resid 10 and name O)	3.94	0.06	0.07
	assign (segid 3A4 and resid 99 and name C) (segid 3A4 and resid 11 and name C)	4.53	0.18	0.18
	assign (segid 3A4 and resid 99 and name C) (segid 3A4 and resid 11 and name CA)	4.43	0.15	0.14
	assign (segid 3A4 and resid 99 and name C) (segid 3A4 and resid 11 and name CB)	5.16	0.13	0.13
	assign (segid 3A4 and resid 99 and name C) (segid 3A4 and resid 11 and name N)	3.26	0.15	0.14
50	assign (segid 3A4 and resid 99 and name C) (segid 3A4 and resid 11 and name O)	5.65	0.21	0.20
	assign (segid 3A4 and resid 99 and name C) (segid 3A4 and resid 12 and name C)	5.08	0.37	0.36
	assign (segid 3A4 and resid 99 and name C) (segid 3A4 and resid 12 and name CA)	4.56	0.19	0.19
	assign (segid 3A4 and resid 99 and name C) (segid 3A4 and resid 12 and name CB)	4.32	0.21	0.21
	assign (segid 3A4 and resid 99 and name C) (segid 3A4 and resid 12 and name N)	3.78	0.19	0.19
55	assign (segid 3A4 and resid 99 and name C) (segid 3A4 and resid 12 and name O)	6.27	0.33	0.34
	assign (segid 3A4 and resid 99 and name C) (segid 3A4 and resid 13 and name CA)	5.46	0.59	0.59
	assign (segid 3A4 and resid 99 and name C) (segid 3A4 and resid 13 and name CB)	5.11	0.66	0.66
	assign (segid 3A4 and resid 99 and name C) (segid 3A4 and resid 13 and name N)	4.48	0.52	0.51
	assign (segid 3A4 and resid 99 and name C) (segid 3A4 and resid 99 and name CB)	2.50	0.03	0.02
60	assign (segid 3A4 and resid 99 and name C) (segid 3A4 and resid 99 and name O)	1.24	0.02	0.01
	assign (segid 3A4 and resid 99 and name CA) (segid 3A4 and resid 10 and name C)	4.41	0.07	0.07
	assign (segid 3A4 and resid 99 and name CA) (segid 3A4 and resid 10 and name CA)	3.83	0.03	0.03
	assign (segid 3A4 and resid 99 and name CA) (segid 3A4 and resid 10 and name CB)	4.91	0.04	0.04
	assign (segid 3A4 and resid 99 and name CA) (segid 3A4 and resid 10 and name N)	2.45	0.03	0.04
65	assign (segid 3A4 and resid 99 and name CA) (segid 3A4 and resid 10 and name O)	5.39	0.07	0.06
	assign (segid 3A4 and resid 99 and name CA) (segid 3A4 and resid 11 and name C)	5.42	0.24	0.25
	assign (segid 3A4 and resid 99 and name CA) (segid 3A4 and resid 11 and name CA)	5.36	0.19	0.20
	assign (segid 3A4 and resid 99 and name CA) (segid 3A4 and resid 11 and name CB)	5.75	0.19	0.19
	assign (segid 3A4 and resid 99 and name CA) (segid 3A4 and resid 11 and name N)	4.32	0.18	0.17
70	assign (segid 3A4 and resid 99 and name CA) (segid 3A4 and resid 11 and name O)	6.57	0.25	0.26
	assign (segid 3A4 and resid 99 and name CA) (segid 3A4 and resid 12 and name C)	5.95	0.45	0.46
	assign (segid 3A4 and resid 99 and name CA) (segid 3A4 and resid 12 and name CA)	5.16	0.33	0.33
	assign (segid 3A4 and resid 99 and name CA) (segid 3A4 and resid 12 and name CB)	4.56	0.40	0.40
	assign (segid 3A4 and resid 99 and name CA) (segid 3A4 and resid 12 and name N)	4.51	0.30	0.31
75	assign (segid 3A4 and resid 99 and name CA) (segid 3A4 and resid 13 and name CA)	6.68	0.65	0.64
	assign (segid 3A4 and resid 99 and name CA) (segid 3A4 and resid 13 and name CB)	6.43	0.71	0.72
	assign (segid 3A4 and resid 99 and name CA) (segid 3A4 and resid 13 and name N)	5.58	0.59	0.58
	assign (segid 3A4 and resid 99 and name CA) (segid 3A4 and resid 19 and name CA)	13.00	1.93	1.93
	assign (segid 3A4 and resid 99 and name CA) (segid 3A4 and resid 19 and name CB)	14.18	2.08	2.07
80	assign (segid 3A4 and resid 99 and name CA) (segid 3A4 and resid 20 and name CA)	14.28	1.24	1.23
	assign (segid 3A4 and resid 99 and name CA) (segid 3A4 and resid 20 and name CB)	15.72	1.26	1.26
	assign (segid 3A4 and resid 99 and name CA) (segid 3A4 and resid 21 and name CA)	13.54	0.97	0.98
	assign (segid 3A4 and resid 99 and name CA) (segid 3A4 and resid 21 and name CB)	12.38	0.96	0.96

	assign (segid 3A4 and resid 9 and name CA) (segid 3A4 and resid 22 and name CA)	14.82	1.05	1.05
	assign (segid 3A4 and resid 9 and name CA) (segid 3A4 and resid 23 and name CA)	13.35	1.14	1.15
	assign (segid 3A4 and resid 9 and name CA) (segid 3A4 and resid 23 and name CB)	12.19	1.24	1.23
	assign (segid 3A4 and resid 9 and name CA) (segid 3A4 and resid 24 and name CA)	15.84	1.35	1.35
	assign (segid 3A4 and resid 9 and name CA) (segid 3A4 and resid 24 and name CB)	16.68	1.35	1.35
5	assign (segid 3A4 and resid 9 and name CA) (segid 3A4 and resid 30 and name CA)	16.71	1.16	1.16
	assign (segid 3A4 and resid 9 and name CA) (segid 3A4 and resid 314 and name CA)	17.38	1.19	1.19
	assign (segid 3A4 and resid 9 and name CA) (segid 3A4 and resid 315 and name CA)	15.53	1.43	1.43
	assign (segid 3A4 and resid 9 and name CA) (segid 3A4 and resid 315 and name CB)	16.34	1.54	1.54
10	assign (segid 3A4 and resid 9 and name CA) (segid 3A4 and resid 316 and name CA)	15.11	1.51	1.50
	assign (segid 3A4 and resid 9 and name CA) (segid 3A4 and resid 317 and name CA)	14.99	0.91	0.92
	assign (segid 3A4 and resid 9 and name CA) (segid 3A4 and resid 318 and name CA)	16.12	1.68	1.68
	assign (segid 3A4 and resid 9 and name CA) (segid 3A4 and resid 318 and name CB)	17.40	1.90	1.91
	assign (segid 3A4 and resid 9 and name CA) (segid 3A4 and resid 319 and name CA)	16.12	1.28	1.28
15	assign (segid 3A4 and resid 9 and name CA) (segid 3A4 and resid 319 and name CB)	17.32	1.19	1.19
	assign (segid 3A4 and resid 9 and name CA) (segid 3A4 and resid 31 and name CA)	15.54	0.89	0.90
	assign (segid 3A4 and resid 9 and name CA) (segid 3A4 and resid 31 and name CB)	16.64	0.83	0.82
	assign (segid 3A4 and resid 9 and name CA) (segid 3A4 and resid 322 and name CA)	18.56	0.83	0.84
	assign (segid 3A4 and resid 9 and name CA) (segid 3A4 and resid 32 and name CA)	12.60	0.79	0.79
20	assign (segid 3A4 and resid 9 and name CA) (segid 3A4 and resid 32 and name CB)	11.26	0.83	0.83
	assign (segid 3A4 and resid 9 and name CA) (segid 3A4 and resid 33 and name CA)	13.51	0.99	0.99
	assign (segid 3A4 and resid 9 and name CA) (segid 3A4 and resid 33 and name CB)	14.78	0.95	0.94
	assign (segid 3A4 and resid 9 and name CA) (segid 3A4 and resid 343 and name CA)	17.71	0.75	0.76
	assign (segid 3A4 and resid 9 and name CA) (segid 3A4 and resid 343 and name CB)	18.40	0.62	0.62
25	assign (segid 3A4 and resid 9 and name CA) (segid 3A4 and resid 344 and name CA)	14.95	0.74	0.74
	assign (segid 3A4 and resid 9 and name CA) (segid 3A4 and resid 344 and name CB)	13.95	0.86	0.86
	assign (segid 3A4 and resid 9 and name CA) (segid 3A4 and resid 345 and name CA)	14.66	0.67	0.66
	assign (segid 3A4 and resid 9 and name CA) (segid 3A4 and resid 345 and name CB)	15.96	0.73	0.73
	assign (segid 3A4 and resid 9 and name CA) (segid 3A4 and resid 346 and name CA)	11.78	0.52	0.51
30	assign (segid 3A4 and resid 9 and name CA) (segid 3A4 and resid 346 and name CB)	10.50	0.42	0.41
	assign (segid 3A4 and resid 9 and name CA) (segid 3A4 and resid 347 and name CA)	13.82	0.47	0.47
	assign (segid 3A4 and resid 9 and name CA) (segid 3A4 and resid 347 and name CB)	14.87	0.41	0.40
	assign (segid 3A4 and resid 9 and name CA) (segid 3A4 and resid 348 and name CA)	11.50	0.32	0.32
	assign (segid 3A4 and resid 9 and name CA) (segid 3A4 and resid 349 and name CA)	10.03	1.23	1.23
35	assign (segid 3A4 and resid 9 and name CA) (segid 3A4 and resid 349 and name CB)	9.53	1.21	1.21
	assign (segid 3A4 and resid 9 and name CA) (segid 3A4 and resid 34 and name CA)	11.24	1.46	1.45
	assign (segid 3A4 and resid 9 and name CA) (segid 3A4 and resid 34 and name CB)	10.17	1.65	1.66
	assign (segid 3A4 and resid 9 and name CA) (segid 3A4 and resid 350 and name CA)	13.41	1.56	1.56
	assign (segid 3A4 and resid 9 and name CA) (segid 3A4 and resid 350 and name CB)	14.46	1.41	1.41
40	assign (segid 3A4 and resid 9 and name CA) (segid 3A4 and resid 351 and name CA)	14.41	1.45	1.45
	assign (segid 3A4 and resid 9 and name CA) (segid 3A4 and resid 352 and name CA)	12.19	1.98	1.98
	assign (segid 3A4 and resid 9 and name CA) (segid 3A4 and resid 352 and name CB)	10.95	1.92	1.91
	assign (segid 3A4 and resid 9 and name CA) (segid 3A4 and resid 353 and name CA)	13.33	2.44	2.44
	assign (segid 3A4 and resid 9 and name CA) (segid 3A4 and resid 353 and name CB)	14.12	2.40	2.40
45	assign (segid 3A4 and resid 9 and name CA) (segid 3A4 and resid 354 and name CA)	15.09	2.75	2.74
	assign (segid 3A4 and resid 9 and name CA) (segid 3A4 and resid 354 and name CB)	14.72	2.85	2.84
	assign (segid 3A4 and resid 9 and name CA) (segid 3A4 and resid 35 and name CA)	13.74	1.92	1.92
	assign (segid 3A4 and resid 9 and name CA) (segid 3A4 and resid 360 and name CA)	14.89	2.23	2.24
	assign (segid 3A4 and resid 9 and name CA) (segid 3A4 and resid 360 and name CB)	13.96	2.29	2.30
50	assign (segid 3A4 and resid 9 and name CA) (segid 3A4 and resid 361 and name CA)	13.73	2.02	2.03
	assign (segid 3A4 and resid 9 and name CA) (segid 3A4 and resid 361 and name CB)	12.94	2.12	2.13
	assign (segid 3A4 and resid 9 and name CA) (segid 3A4 and resid 382 and name CB)	18.23	1.14	1.14
	assign (segid 3A4 and resid 9 and name CA) (segid 3A4 and resid 383 and name CA)	18.56	0.82	0.83
55	assign (segid 3A4 and resid 9 and name CA) (segid 3A4 and resid 38 and name CB)	17.00	1.64	1.63
	assign (segid 3A4 and resid 9 and name CA) (segid 3A4 and resid 39 and name CB)	16.45	1.28	1.28
	assign (segid 3A4 and resid 9 and name CA) (segid 3A4 and resid 429 and name CA)	13.96	2.36	2.37
	assign (segid 3A4 and resid 9 and name CA) (segid 3A4 and resid 430 and name CA)	14.02	1.28	1.28
	assign (segid 3A4 and resid 9 and name CA) (segid 3A4 and resid 431 and name CA)	15.90	1.30	1.30
	assign (segid 3A4 and resid 9 and name CA) (segid 3A4 and resid 433 and name CA)	14.95	1.76	1.77
60	assign (segid 3A4 and resid 9 and name C)	1.53	0.01	0.00
	assign (segid 3A4 and resid 9 and name CB)	1.52	0.02	0.01
	assign (segid 3A4 and resid 9 and name O)	2.39	0.02	0.02
	assign (segid 3A4 and resid 10 and name C)	5.45	0.05	0.05
	assign (segid 3A4 and resid 10 and name CA)	4.52	0.07	0.07
65	assign (segid 3A4 and resid 10 and name CB)	5.41	0.12	0.12
	assign (segid 3A4 and resid 10 and name N)	3.19	0.09	0.08
	assign (segid 3A4 and resid 10 and name O)	6.39	0.07	0.07
	assign (segid 3A4 and resid 11 and name C)	6.82	0.26	0.26
	assign (segid 3A4 and resid 11 and name CA)	6.73	0.16	0.16
70	assign (segid 3A4 and resid 11 and name CB)	7.18	0.15	0.15
	assign (segid 3A4 and resid 11 and name N)	5.57	0.13	0.12
	assign (segid 3A4 and resid 12 and name CA)	6.42	0.39	0.40
	assign (segid 3A4 and resid 12 and name CB)	5.67	0.49	0.49
	assign (segid 3A4 and resid 12 and name N)	5.90	0.33	0.33
75	assign (segid 3A4 and resid 13 and name CA)	7.49	0.74	0.73
	assign (segid 3A4 and resid 13 and name CB)	7.02	0.84	0.83
	assign (segid 3A4 and resid 19 and name CA)	13.97	1.88	1.87
	assign (segid 3A4 and resid 19 and name CB)	15.19	2.02	2.01
	assign (segid 3A4 and resid 20 and name CA)	14.97	1.18	1.19
80	assign (segid 3A4 and resid 20 and name CB)	16.41	1.19	1.20
	assign (segid 3A4 and resid 21 and name CA)	14.01	1.05	1.04
	assign (segid 3A4 and resid 21 and name CB)	12.86	1.03	1.04
	assign (segid 3A4 and resid 22 and name CA)	14.96	1.26	1.27

	assign (segid 3A4 and resid 9 and name CB) (segid 3A4 and resid 23 and name CA)	13.18	1.55	1.54
	assign (segid 3A4 and resid 9 and name CB) (segid 3A4 and resid 23 and name CB)	11.98	1.63	1.63
	assign (segid 3A4 and resid 9 and name CB) (segid 3A4 and resid 24 and name CA)	15.40	1.82	1.83
	assign (segid 3A4 and resid 9 and name CB) (segid 3A4 and resid 30 and name CA)	16.60	1.53	1.54
5	assign (segid 3A4 and resid 9 and name CB) (segid 3A4 and resid 315 and name CA)	16.07	1.68	1.68
	assign (segid 3A4 and resid 9 and name CB) (segid 3A4 and resid 316 and name CA)	15.40	1.58	1.59
	assign (segid 3A4 and resid 9 and name CB) (segid 3A4 and resid 317 and name CA)	15.30	1.00	0.99
	assign (segid 3A4 and resid 9 and name CB) (segid 3A4 and resid 318 and name CA)	16.15	1.70	1.71
	assign (segid 3A4 and resid 9 and name CB) (segid 3A4 and resid 318 and name CB)	17.40	1.95	1.94
10	assign (segid 3A4 and resid 9 and name CB) (segid 3A4 and resid 319 and name CA)	16.13	1.25	1.26
	assign (segid 3A4 and resid 9 and name CB) (segid 3A4 and resid 319 and name CB)	17.35	1.18	1.18
	assign (segid 3A4 and resid 9 and name CB) (segid 3A4 and resid 31 and name CA)	15.73	1.15	1.15
	assign (segid 3A4 and resid 9 and name CB) (segid 3A4 and resid 31 and name CB)	16.89	1.03	1.03
	assign (segid 3A4 and resid 9 and name CB) (segid 3A4 and resid 32 and name CA)	12.93	1.01	1.01
15	assign (segid 3A4 and resid 9 and name CB) (segid 3A4 and resid 32 and name CB)	11.55	1.10	1.11
	assign (segid 3A4 and resid 9 and name CB) (segid 3A4 and resid 33 and name CA)	14.13	0.97	0.97
	assign (segid 3A4 and resid 9 and name CB) (segid 3A4 and resid 33 and name CB)	15.39	0.90	0.91
	assign (segid 3A4 and resid 9 and name CB) (segid 3A4 and resid 343 and name CA)	17.87	0.98	0.97
	assign (segid 3A4 and resid 9 and name CB) (segid 3A4 and resid 344 and name CA)	15.08	0.95	0.95
20	assign (segid 3A4 and resid 9 and name CB) (segid 3A4 and resid 344 and name CB)	13.99	1.14	1.15
	assign (segid 3A4 and resid 9 and name CB) (segid 3A4 and resid 345 and name CA)	15.04	0.55	0.55
	assign (segid 3A4 and resid 9 and name CB) (segid 3A4 and resid 345 and name CB)	16.37	0.55	0.55
	assign (segid 3A4 and resid 9 and name CB) (segid 3A4 and resid 346 and name CA)	12.22	0.42	0.43
	assign (segid 3A4 and resid 9 and name CB) (segid 3A4 and resid 346 and name CB)	10.98	0.42	0.42
25	assign (segid 3A4 and resid 9 and name CB) (segid 3A4 and resid 347 and name CA)	14.33	0.38	0.38
	assign (segid 3A4 and resid 9 and name CB) (segid 3A4 and resid 347 and name CB)	15.30	0.19	0.18
	assign (segid 3A4 and resid 9 and name CB) (segid 3A4 and resid 348 and name CA)	12.05	0.59	0.58
	assign (segid 3A4 and resid 9 and name CB) (segid 3A4 and resid 349 and name CA)	10.85	1.47	1.48
	assign (segid 3A4 and resid 9 and name CB) (segid 3A4 and resid 349 and name CB)	10.36	1.41	1.42
30	assign (segid 3A4 and resid 9 and name CB) (segid 3A4 and resid 34 and name CA)	12.10	1.49	1.48
	assign (segid 3A4 and resid 9 and name CB) (segid 3A4 and resid 34 and name CB)	11.08	1.69	1.69
	assign (segid 3A4 and resid 9 and name CB) (segid 3A4 and resid 350 and name CA)	14.28	1.73	1.73
	assign (segid 3A4 and resid 9 and name CB) (segid 3A4 and resid 350 and name CB)	15.28	1.55	1.54
	assign (segid 3A4 and resid 9 and name CB) (segid 3A4 and resid 351 and name CA)	15.23	1.74	1.74
35	assign (segid 3A4 and resid 9 and name CB) (segid 3A4 and resid 352 and name CA)	13.13	2.35	2.35
	assign (segid 3A4 and resid 9 and name CB) (segid 3A4 and resid 352 and name CB)	11.84	2.30	2.30
	assign (segid 3A4 and resid 9 and name CB) (segid 3A4 and resid 353 and name CA)	14.43	2.69	2.70
	assign (segid 3A4 and resid 9 and name CB) (segid 3A4 and resid 353 and name CB)	15.21	2.61	2.62
	assign (segid 3A4 and resid 9 and name CB) (segid 3A4 and resid 35 and name CA)	14.75	1.94	1.93
40	assign (segid 3A4 and resid 9 and name CB) (segid 3A4 and resid 360 and name CB)	14.93	2.76	2.76
	assign (segid 3A4 and resid 9 and name CB) (segid 3A4 and resid 361 and name CA)	14.49	2.55	2.55
	assign (segid 3A4 and resid 9 and name CB) (segid 3A4 and resid 361 and name CB)	13.70	2.67	2.66
	assign (segid 3A4 and resid 9 and name CB) (segid 3A4 and resid 39 and name CB)	17.16	1.27	1.27
	assign (segid 3A4 and resid 9 and name CB) (segid 3A4 and resid 429 and name CA)	13.25	2.44	2.44
45	assign (segid 3A4 and resid 9 and name CB) (segid 3A4 and resid 430 and name CA)	13.38	1.56	1.57
	assign (segid 3A4 and resid 9 and name CB) (segid 3A4 and resid 431 and name CA)	15.44	1.31	1.31
	assign (segid 3A4 and resid 9 and name CB) (segid 3A4 and resid 433 and name CA)	14.62	1.76	1.76
	assign (segid 3A4 and resid 9 and name CB) (segid 3A4 and resid 10 and name C)	4.68	0.04	0.03
	assign (segid 3A4 and resid 9 and name N) (segid 3A4 and resid 10 and name CB)	4.23	0.05	0.04
50	assign (segid 3A4 and resid 9 and name N) (segid 3A4 and resid 10 and name N)	5.04	0.07	0.06
	assign (segid 3A4 and resid 9 and name N) (segid 3A4 and resid 10 and name N)	2.83	0.06	0.05
	assign (segid 3A4 and resid 9 and name N) (segid 3A4 and resid 10 and name O)	5.80	0.03	0.04
	assign (segid 3A4 and resid 9 and name N) (segid 3A4 and resid 11 and name C)	5.55	0.13	0.13
	assign (segid 3A4 and resid 9 and name N) (segid 3A4 and resid 11 and name CA)	5.21	0.10	0.10
55	assign (segid 3A4 and resid 9 and name N) (segid 3A4 and resid 11 and name CB)	5.24	0.12	0.11
	assign (segid 3A4 and resid 9 and name N) (segid 3A4 and resid 11 and name N)	4.24	0.10	0.09
	assign (segid 3A4 and resid 9 and name N) (segid 3A4 and resid 11 and name O)	6.75	0.12	0.12
	assign (segid 3A4 and resid 9 and name N) (segid 3A4 and resid 12 and name C)	6.68	0.34	0.35
	assign (segid 3A4 and resid 9 and name N) (segid 3A4 and resid 12 and name CA)	5.69	0.24	0.24
60	assign (segid 3A4 and resid 9 and name N) (segid 3A4 and resid 12 and name CB)	5.26	0.37	0.37
	assign (segid 3A4 and resid 9 and name N) (segid 3A4 and resid 12 and name N)	4.82	0.20	0.20
	assign (segid 3A4 and resid 9 and name N) (segid 3A4 and resid 13 and name N)	6.43	0.44	0.44
	assign (segid 3A4 and resid 9 and name N) (segid 3A4 and resid 9 and name C)	2.45	0.02	0.02
	assign (segid 3A4 and resid 9 and name N) (segid 3A4 and resid 9 and name CA)	1.46	0.01	0.00
65	assign (segid 3A4 and resid 9 and name N) (segid 3A4 and resid 9 and name CB)	2.46	0.02	0.01
	assign (segid 3A4 and resid 9 and name N) (segid 3A4 and resid 9 and name O)	3.49	0.05	0.04
	assign (segid 3A4 and resid 9 and name O) (segid 3A4 and resid 10 and name C)	3.02	0.07	0.06
	assign (segid 3A4 and resid 9 and name O) (segid 3A4 and resid 10 and name CA)	2.75	0.02	0.03
	assign (segid 3A4 and resid 9 and name O) (segid 3A4 and resid 10 and name CB)	4.25	0.03	0.02
70	assign (segid 3A4 and resid 9 and name O) (segid 3A4 and resid 10 and name N)	2.24	0.00	0.01
	assign (segid 3A4 and resid 9 and name O) (segid 3A4 and resid 10 and name O)	3.58	0.10	0.09
	assign (segid 3A4 and resid 9 and name O) (segid 3A4 and resid 11 and name C)	4.12	0.19	0.19
	assign (segid 3A4 and resid 9 and name O) (segid 3A4 and resid 11 and name CA)	4.38	0.14	0.15
	assign (segid 3A4 and resid 9 and name O) (segid 3A4 and resid 11 and name CB)	5.34	0.13	0.14
75	assign (segid 3A4 and resid 9 and name O) (segid 3A4 and resid 11 and name N)	3.44	0.13	0.13
	assign (segid 3A4 and resid 9 and name O) (segid 3A4 and resid 11 and name O)	5.10	0.24	0.24
	assign (segid 3A4 and resid 9 and name O) (segid 3A4 and resid 12 and name C)	4.05	0.38	0.38
	assign (segid 3A4 and resid 9 and name O) (segid 3A4 and resid 12 and name CA)	3.76	0.16	0.16
	assign (segid 3A4 and resid 9 and name O) (segid 3A4 and resid 12 and name CB)	3.52	0.12	0.13
	assign (segid 3A4 and resid 9 and name O) (segid 3A4 and resid 12 and name N)	3.25	0.18	0.18
80	assign (segid 3A4 and resid 9 and name O) (segid 3A4 and resid 12 and name O)	5.22	0.34	0.34
	assign (segid 3A4 and resid 9 and name O) (segid 3A4 and resid 13 and name C)	5.51	0.68	0.68
	assign (segid 3A4 and resid 9 and name O) (segid 3A4 and resid 13 and name CA)	4.36	0.67	0.68

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TABLE 4

10	assign	(resid 6 and name N)	(resid 6 and name N)	(resid 6 and name CA)		
		(resid 6 and name C)	(resid 7 and name N)	1 -35.9	16.2	2
	assign	(resid 6 and name C)	(resid 7 and name N)			
		(resid 7 and name CA)	(resid 7 and name C)	1 -64.1	7.1	2
	assign	(resid 7 and name N)	(resid 7 and name CA)			
		(resid 7 and name C)	(resid 8 and name N)	1 -34.4	22.5	2
15	assign	(resid 7 and name C)	(resid 8 and name N)			
		(resid 8 and name CA)	(resid 8 and name C)	1 -66.5	18.2	2
	assign	(resid 8 and name N)	(resid 8 and name CA)			
		(resid 8 and name C)	(resid 9 and name N)	1 -37.2	13.2	2
	assign	(resid 8 and name C)	(resid 9 and name N)			
		(resid 9 and name CA)	(resid 9 and name C)	1 -69.8	26.1	2
20	assign	(resid 9 and name N)	(resid 9 and name CA)			
		(resid 9 and name C)	(resid 10 and name N)	1 -40.8	20.3	2
	assign	(resid 9 and name C)	(resid 10 and name N)			
		(resid 10 and name CA)	(resid 10 and name C)	1 -66.3	5.1	2
25	assign	(resid 10 and name N)	(resid 10 and name CA)			
		(resid 10 and name C)	(resid 11 and name N)	1 -35.4	14.1	2
	assign	(resid 10 and name C)	(resid 11 and name N)			
		(resid 11 and name CA)	(resid 11 and name C)	1 -65.9	20.1	2
30	assign	(resid 11 and name N)	(resid 11 and name CA)			
		(resid 11 and name C)	(resid 12 and name N)	1 -33.8	27.1	2
	assign	(resid 11 and name C)	(resid 12 and name N)			
		(resid 12 and name CA)	(resid 12 and name C)	1 -61.9	11.1	2
	assign	(resid 12 and name N)	(resid 12 and name CA)			
		(resid 12 and name C)	(resid 13 and name N)	1 -41.0	13.3	2
35	assign	(resid 12 and name C)	(resid 13 and name N)			
		(resid 13 and name CA)	(resid 13 and name C)	1 -65.3	21.4	2
	assign	(resid 19 and name N)	(resid 19 and name CA)			
		(resid 19 and name C)	(resid 20 and name N)	1 -28.8	21.6	2
40	assign	(resid 19 and name C)	(resid 20 and name N)			
		(resid 20 and name CA)	(resid 20 and name C)	1 -135.9	26.0	2
	assign	(resid 20 and name N)	(resid 20 and name CA)			
		(resid 20 and name C)	(resid 21 and name N)	1 117.1	21.0	2
	assign	(resid 20 and name C)	(resid 21 and name N)			
		(resid 21 and name CA)	(resid 21 and name C)	1 -140.2	15.2	2
45	assign	(resid 21 and name N)	(resid 21 and name CA)			
		(resid 21 and name C)	(resid 22 and name N)	1 161.8	24.1	2
	assign	(resid 21 and name C)	(resid 22 and name N)			
		(resid 22 and name CA)	(resid 22 and name C)	1 -100.1	37.5	2
50	assign	(resid 22 and name N)	(resid 22 and name CA)			
		(resid 22 and name C)	(resid 23 and name N)	1 141.1	15.3	2
	assign	(resid 22 and name C)	(resid 23 and name N)			
		(resid 23 and name CA)	(resid 23 and name C)	1 -127.3	23.5	2
	assign	(resid 23 and name N)	(resid 23 and name CA)			
		(resid 23 and name C)	(resid 24 and name N)	1 155.6	31.5	2
55	assign	(resid 23 and name C)	(resid 24 and name N)			
		(resid 24 and name CA)	(resid 24 and name C)	1 -118.5	36.1	2
	assign	(resid 24 and name C)	(resid 25 and name N)			
		(resid 25 and name CA)	(resid 25 and name C)	1 -106.7	58.4	2
	assign	(resid 25 and name N)	(resid 25 and name CA)			
		(resid 25 and name C)	(resid 26 and name N)	1 141.5	84.7	2
60	assign	(resid 29 and name N)	(resid 29 and name CA)			
		(resid 29 and name C)	(resid 30 and name N)	1 135.8	20.2	2
	assign	(resid 29 and name C)	(resid 30 and name N)			
		(resid 30 and name CA)	(resid 30 and name C)	1 -146.2	27.9	2
65	assign	(resid 30 and name N)	(resid 30 and name CA)			
		(resid 30 and name C)	(resid 31 and name N)	1 149.4	42.7	2
	assign	(resid 30 and name C)	(resid 31 and name N)			
		(resid 31 and name CA)	(resid 31 and name C)	1 -95.8		

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assign (resid 33 and name C) (resid 34 and name N)
(resid 34 and name CA) (resid 34 and name C) 1 -112.8 21.3 2
assign (resid 34 and name N) (resid 34 and name CA)
(resid 34 and name C) (resid 35 and name N) 1 -20.8 27.2 2
5 assign (resid 34 and name C) (resid 35 and name N)
(resid 35 and name CA) (resid 35 and name C) 1 -91.0 40.5 2
assign (resid 35 and name N) (resid 35 and name CA)
(resid 35 and name C) (resid 36 and name N) 1 150.2 20.8 2
10 assign (resid 36 and name N) (resid 36 and name CA)
(resid 36 and name C) (resid 37 and name N) 1 -42.1 16.7 2
assign (resid 36 and name C) (resid 37 and name N)
(resid 37 and name CA) (resid 37 and name C) 1 -60.6 12.0 2
assign (resid 37 and name N) (resid 37 and name CA)
(resid 37 and name C) (resid 38 and name N) 1 -43.6 11.6 2
15 assign (resid 37 and name C) (resid 38 and name N)
(resid 38 and name CA) (resid 38 and name C) 1 -71.0 15.2 2
assign (resid 38 and name N) (resid 38 and name CA)
(resid 38 and name C) (resid 39 and name N) 1 -37.5 12.3 2
20 assign (resid 38 and name C) (resid 39 and name N)
(resid 39 and name CA) (resid 39 and name C) 1 -66.8 10.0 2
assign (resid 39 and name N) (resid 39 and name CA)
(resid 39 and name C) (resid 40 and name N) 1 -45.2 9.2 2
assign (resid 39 and name C) (resid 40 and name N)
(resid 40 and name CA) (resid 40 and name C) 1 -60.5 3.8 2
25 assign (resid 40 and name N) (resid 40 and name CA)
(resid 40 and name C) (resid 41 and name N) 1 -41.0 17.3 2
assign (resid 40 and name C) (resid 41 and name N)
(resid 41 and name CA) (resid 41 and name C) 1 -63.8 19.6 2
30 assign (resid 41 and name N) (resid 41 and name CA)
(resid 41 and name C) (resid 42 and name N) 1 -45.4 5.8 2
assign (resid 41 and name C) (resid 42 and name N)
(resid 42 and name CA) (resid 42 and name C) 1 -64.6 8.5 2
assign (resid 42 and name N) (resid 42 and name CA)
(resid 42 and name C) (resid 43 and name N) 1 164.9 13.0 2
35 assign (resid 43 and name N) (resid 43 and name CA)
(resid 43 and name C) (resid 44 and name N) 1 -67.1 53.3 2
assign (resid 44 and name N) (resid 44 and name CA)
(resid 44 and name C) (resid 45 and name N) 1 -45.8 11.4 2
40 assign (resid 45 and name N) (resid 45 and name CA)
(resid 45 and name C) (resid 46 and name N) 1 -49.0 25.7 2
assign (resid 46 and name N) (resid 46 and name CA)
(resid 46 and name C) (resid 47 and name N) 1 -63.6 33.9 2
45 assign (resid 47 and name N) (resid 47 and name CA)
(resid 47 and name C) (resid 48 and name N) 1 -35.0 13.9 2
assign (resid 48 and name N) (resid 48 and name CA)
(resid 48 and name C) (resid 49 and name N) 1 -70.5 28.8 2
50 assign (resid 49 and name N) (resid 49 and name CA)
(resid 49 and name C) (resid 50 and name N) 1 -65.7 37.1 2
assign (resid 50 and name N) (resid 50 and name CA)
(resid 50 and name C) (resid 51 and name N) 1 -30.2 33.1 2
55 assign (resid 51 and name N) (resid 51 and name CA)
(resid 51 and name C) (resid 52 and name N) 1 -75.2 19.4 2
assign (resid 52 and name N) (resid 52 and name CA)
(resid 52 and name C) (resid 53 and name N) 1 154.2 29.4 2
60 assign (resid 53 and name N) (resid 53 and name CA)
(resid 53 and name C) (resid 54 and name N) 1 -96.5 30.8 2
assign (resid 54 and name N) (resid 54 and name CA)
(resid 54 and name C) (resid 55 and name N) 1 154.8 20.8 2
65 assign (resid 55 and name N) (resid 55 and name CA)
(resid 55 and name C) (resid 56 and name N) 1 -59.7 18.1 2
assign (resid 56 and name N) (resid 56 and name CA)
(resid 56 and name C) (resid 57 and name N) 1 -78.2 35.2 2
70 assign (resid 57 and name N) (resid 57 and name CA)
(resid 57 and name C) (resid 58 and name N) 1 -19.7 36.4 2
assign (resid 58 and name N) (resid 58 and name CA)
(resid 58 and name C) (resid 59 and name N) 1 -68.3 36.1 2
75 assign (resid 59 and name N) (resid 59 and name CA)
(resid 59 and name C) (resid 60 and name N) 1 -36.6 23.9 2
assign (resid 60 and name N) (resid 60 and name CA)
(resid 60 and name C) (resid 61 and name N) 1 -58.1 10.1 2
80 assign (resid 61 and name N) (resid 61 and name CA)
(resid 61 and name C) (resid 62 and name N) 1 -55.2 33.4 2
assign (resid 62 and name N) (resid 62 and name CA)
(resid 62 and name C) (resid 63 and name N) 1 -53.5 26.2 2
assign (resid 63 and name N) (resid 63 and name CA)
(resid 63 and name C) (resid 64 and name N) 1 -41.0 15.3 2
assign (resid 64 and name N) (resid 64 and name CA)
(resid 64 and name C) (resid 65 and name N) 1 -69.2 5.8 2
85 assign (resid 65 and name N) (resid 65 and name CA)
(resid 65 and name C) (resid 66 and name N) 1 -45.5 15.4 2
assign (resid 66 and name N) (resid 66 and name CA)
(resid 66 and name C) (resid 67 and name N) 1 -68.5 13.0 2
assign (resid 67 and name N) (resid 67 and name CA)

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5  assign (resid 78 and name C) (resid 79 and name N) 1 -39.4 19.0 2
    assign (resid 78 and name C) (resid 79 and name C) 1 -63.8 13.2 2
    assign (resid 79 and name N) (resid 79 and name CA) 1 -44.0 17.1 2
    assign (resid 79 and name C) (resid 80 and name N) 1 -57.8 13.3 2
    assign (resid 80 and name CA) (resid 80 and name C) 1 -40.1 26.3 2
10  assign (resid 80 and name N) (resid 81 and name N) 1 -64.0 15.2 2
    assign (resid 81 and name CA) (resid 81 and name C) 1 -41.2 12.0 2
    assign (resid 81 and name N) (resid 82 and name N) 1 -82.3 39.9 2
15  assign (resid 82 and name CA) (resid 82 and name C) 1 -30.5 27.7 2
    assign (resid 82 and name C) (resid 83 and name N) 1 -53.0 16.2 2
    assign (resid 83 and name CA) (resid 83 and name C) 1 -38.9 17.2 2
20  assign (resid 83 and name N) (resid 84 and name N) 1 -35.0 25.9 2
    assign (resid 84 and name C) (resid 85 and name N) 1 -79.3 29.7 2
    assign (resid 85 and name CA) (resid 85 and name C) 1 -27.4 20.9 2
25  assign (resid 85 and name N) (resid 86 and name N) 1 -96.8 24.7 2
    assign (resid 86 and name C) (resid 86 and name C) 1 -18.1 28.6 2
    assign (resid 94 and name N) (resid 94 and name CA) 1 -56.2 13.2 2
30  assign (resid 95 and name N) (resid 95 and name CA) 1 -45.0 12.2 2
    assign (resid 95 and name C) (resid 96 and name N) 1 -35.1 22.6 2
    assign (resid 96 and name CA) (resid 97 and name N) 1 -70.0 21.8 2
35  assign (resid 97 and name N) (resid 97 and name C) 1 -39.1 24.2 2
    assign (resid 97 and name C) (resid 98 and name N) 1 -60.4 14.1 2
    assign (resid 98 and name CA) (resid 98 and name C) 1 -43.0 13.7 2
40  assign (resid 98 and name N) (resid 99 and name N) 1 -63.3 6.3 2
    assign (resid 99 and name CA) (resid 99 and name C) 1 -38.9 9.9 2
    assign (resid 99 and name N) (resid 100 and name N) 1 -62.5 8.3 2
45  assign (resid 100 and name CA) (resid 100 and name C) 1 -46.3 9.3 2
    assign (resid 100 and name N) (resid 101 and name N) 1 -65.0 14.8 2
    assign (resid 101 and name CA) (resid 101 and name C) 1 -40.8 10.6 2
50  assign (resid 101 and name N) (resid 102 and name N) 1 -61.3 7.7 2
    assign (resid 102 and name CA) (resid 102 and name C) 1 -41.8 11.6 2
    assign (resid 102 and name N) (resid 103 and name N) 1 -65.7 9.2 2
55  assign (resid 103 and name CA) (resid 103 and name C) 1 -42.8 7.4 2
    assign (resid 103 and name N) (resid 104 and name N) 1 -61.8 7.8 2
    assign (resid 104 and name CA) (resid 104 and name C) 1 -41.6 7.2 2
60  assign (resid 104 and name N) (resid 105 and name N) 1 -65.7 7.8 2
    assign (resid 105 and name CA) (resid 105 and name C) 1 -41.6 14.3 2
    assign (resid 105 and name N) (resid 106 and name N) 1 -65.9 10.6 2
65  assign (resid 106 and name CA) (resid 106 and name C) 1 -44.3 5.5 2
    assign (resid 106 and name N) (resid 107 and name N) 1 -60.0 5.8 2
    assign (resid 107 and name CA) (resid 107 and name C) 1 -44.5 20.1 2
70  assign (resid 107 and name N) (resid 108 and name N) 1 -60.2 9.1 2
    assign (resid 108 and name CA) (resid 108 and name C) 1 -60.2 9.1 2

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assign (resid 108 and name N) (resid 108 and name CA)
      (resid 108 and name C) (resid 109 and name N) 1 -38.8 20.5 2
assign (resid 108 and name C) (resid 109 and name N)
      (resid 109 and name CA) (resid 109 and name C) 1 -72.3 14.4 2
5 assign (resid 109 and name N) (resid 109 and name CA)
      (resid 109 and name C) (resid 110 and name N) 1 -35.4 13.5 2
assign (resid 109 and name C) (resid 110 and name N)
      (resid 110 and name CA) (resid 110 and name C) 1 -59.3 26.8 2
10 assign (resid 110 and name N) (resid 110 and name CA)
      (resid 110 and name C) (resid 111 and name N) 1 -36.7 24.8 2
assign (resid 110 and name C) (resid 111 and name N)
      (resid 111 and name CA) (resid 111 and name C) 1 -76.2 23.8 2
assign (resid 111 and name N) (resid 111 and name CA)
      (resid 111 and name C) (resid 112 and name N) 1 2.0 45.0 2
15 assign (resid 111 and name C) (resid 112 and name N)
      (resid 112 and name CA) (resid 112 and name C) 1 -92.8 70.2 2
assign (resid 119 and name C) (resid 120 and name N)
      (resid 120 and name CA) (resid 120 and name C) 1 -96.9 17.5 2
20 assign (resid 120 and name N) (resid 120 and name CA)
      (resid 120 and name C) (resid 121 and name N) 1 102.1 23.8 2
assign (resid 120 and name C) (resid 121 and name N)
      (resid 121 and name CA) (resid 121 and name C) 1 -58.6 17.3 2
assign (resid 121 and name N) (resid 121 and name CA)
      (resid 121 and name C) (resid 122 and name N) 1 -31.7 26.0 2
25 assign (resid 121 and name C) (resid 122 and name N)
      (resid 122 and name CA) (resid 122 and name C) 1 -64.1 21.7 2
assign (resid 122 and name N) (resid 122 and name CA)
      (resid 122 and name C) (resid 123 and name N) 1 -51.5 25.4 2
30 assign (resid 122 and name C) (resid 123 and name N)
      (resid 123 and name CA) (resid 123 and name C) 1 -69.8 10.8 2
assign (resid 123 and name N) (resid 123 and name CA)
      (resid 123 and name C) (resid 124 and name N) 1 -41.3 35.6 2
assign (resid 123 and name C) (resid 124 and name N)
      (resid 124 and name CA) (resid 124 and name C) 1 -78.5 29.8 2
35 assign (resid 124 and name N) (resid 124 and name CA)
      (resid 124 and name C) (resid 125 and name N) 1 -21.4 17.3 2
assign (resid 124 and name C) (resid 125 and name N)
      (resid 125 and name CA) (resid 125 and name C) 1 -119.8 69.2 2
40 assign (resid 125 and name N) (resid 125 and name CA)
      (resid 125 and name C) (resid 126 and name N) 1 -50.0 42.1 2
assign (resid 125 and name C) (resid 126 and name N)
      (resid 126 and name CA) (resid 126 and name C) 1 -65.6 33.2 2
45 assign (resid 126 and name N) (resid 126 and name CA)
      (resid 126 and name C) (resid 127 and name N) 1 -29.0 17.1 2
assign (resid 126 and name C) (resid 127 and name N)
      (resid 127 and name CA) (resid 127 and name C) 1 -73.0 14.1 2
50 assign (resid 127 and name N) (resid 127 and name CA)
      (resid 127 and name C) (resid 128 and name N) 1 -49.3 16.7 2
assign (resid 127 and name C) (resid 128 and name N)
      (resid 128 and name CA) (resid 128 and name C) 1 -64.0 26.8 2
55 assign (resid 128 and name N) (resid 128 and name CA)
      (resid 128 and name C) (resid 129 and name N) 1 -44.4 10.4 2
assign (resid 128 and name C) (resid 129 and name N)
      (resid 129 and name CA) (resid 129 and name C) 1 -57.0 18.5 2
60 assign (resid 129 and name N) (resid 129 and name CA)
      (resid 129 and name C) (resid 130 and name N) 1 -54.6 26.4 2
assign (resid 129 and name C) (resid 130 and name N)
      (resid 130 and name CA) (resid 130 and name C) 1 -63.6 8.6 2
65 assign (resid 130 and name N) (resid 130 and name CA)
      (resid 130 and name C) (resid 131 and name N) 1 -35.7 12.2 2
assign (resid 130 and name C) (resid 131 and name N)
      (resid 131 and name CA) (resid 131 and name C) 1 -67.8 6.2 2
70 assign (resid 131 and name N) (resid 131 and name CA)
      (resid 131 and name C) (resid 132 and name N) 1 -44.1 16.1 2
assign (resid 131 and name C) (resid 132 and name N)
      (resid 132 and name CA) (resid 132 and name C) 1 -61.2 8.1 2
75 assign (resid 132 and name N) (resid 132 and name CA)
      (resid 132 and name C) (resid 133 and name N) 1 -40.6 10.4 2
assign (resid 132 and name C) (resid 133 and name N)
      (resid 133 and name CA) (resid 133 and name C) 1 -66.7 9.0 2
80 assign (resid 133 and name N) (resid 133 and name CA)
      (resid 133 and name C) (resid 134 and name N) 1 -44.0 17.7 2
assign (resid 133 and name C) (resid 134 and name N)
      (resid 134 and name CA) (resid 134 and name C) 1 -63.8 8.3 2
assign (resid 134 and name N) (resid 134 and name CA)
      (resid 134 and name C) (resid 135 and name N) 1 -39.4 10.2 2
assign (resid 134 and name C) (resid 135 and name N)
      (resid 135 and name CA) (resid 135 and name C) 1 -66.5 15.7 2
assign (resid 135 and name N) (resid 135 and name CA)
      (resid 135 and name C) (resid 136 and name N) 1 -41.4 13.1 2
assign (resid 135 and name C) (resid 136 and name N)
      (resid 136 and name CA) (resid 136 and name C) 1 -69.1 16.9 2
assign (resid 136 and name N) (resid 136 and name CA)

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      (resid 136 and name C) (resid 137 and name N) 1 -33.5 27.3 2
assign (resid 136 and name C) (resid 137 and name N)
      (resid 137 and name CA) (resid 137 and name C) 1 -74.7 38.0 2
5 assign (resid 137 and name N) (resid 137 and name CA)
      (resid 137 and name C) (resid 138 and name N) 1 -41.3 24.7 2
assign (resid 137 and name C) (resid 138 and name N)
      (resid 138 and name CA) (resid 138 and name C) 1 -94.8 51.9 2
assign (resid 138 and name N) (resid 138 and name CA)
      (resid 138 and name C) (resid 139 and name N) 1 -17.5 48.8 2
10 assign (resid 138 and name C) (resid 139 and name N)
      (resid 139 and name CA) (resid 139 and name C) 1 89.3 54.2 2
assign (resid 139 and name N) (resid 139 and name CA)
      (resid 139 and name C) (resid 140 and name N) 1 19.5 40.1 2
15 assign (resid 139 and name C) (resid 140 and name N)
      (resid 140 and name CA) (resid 140 and name C) 1 -93.3 37.3 2
assign (resid 140 and name N) (resid 140 and name CA)
      (resid 140 and name C) (resid 141 and name N) 1 138.9 30.9 2
assign (resid 140 and name C) (resid 141 and name N)
      (resid 141 and name CA) (resid 141 and name C) 1 -85.4 53.6 2
20 assign (resid 147 and name N) (resid 147 and name CA)
      (resid 147 and name C) (resid 148 and name N) 1 -43.4 28.0 2
assign (resid 148 and name N) (resid 148 and name CA)
      (resid 148 and name C) (resid 149 and name N) 1 -10.2 79.0 2
25 assign (resid 149 and name N) (resid 149 and name CA)
      (resid 149 and name C) (resid 150 and name N) 1 -23.2 50.0 2
assign (resid 149 and name C) (resid 150 and name N)
      (resid 150 and name CA) (resid 150 and name C) 1 -54.0 10.8 2
30 assign (resid 151 and name N) (resid 151 and name CA)
      (resid 151 and name C) (resid 152 and name N) 1 -47.9 6.4 2
assign (resid 151 and name C) (resid 152 and name N)
      (resid 152 and name CA) (resid 152 and name C) 1 -61.9 18.9 2
35 assign (resid 152 and name N) (resid 152 and name CA)
      (resid 152 and name C) (resid 153 and name N) 1 -47.4 18.9 2
assign (resid 152 and name C) (resid 153 and name N)
      (resid 153 and name CA) (resid 153 and name C) 1 -64.0 11.8 2
40 assign (resid 153 and name N) (resid 153 and name CA)
      (resid 153 and name C) (resid 154 and name N) 1 -36.0 19.8 2
assign (resid 153 and name C) (resid 154 and name N)
      (resid 154 and name CA) (resid 154 and name C) 1 -62.0 18.2 2
45 assign (resid 154 and name N) (resid 154 and name CA)
      (resid 154 and name C) (resid 155 and name N) 1 -41.2 8.0 2
assign (resid 154 and name C) (resid 155 and name N)
      (resid 155 and name CA) (resid 155 and name C) 1 -65.3 6.6 2
50 assign (resid 155 and name N) (resid 155 and name CA)
      (resid 155 and name C) (resid 156 and name N) 1 -45.5 23.3 2
assign (resid 155 and name C) (resid 156 and name N)
      (resid 156 and name CA) (resid 156 and name C) 1 -58.6 18.5 2
55 assign (resid 156 and name N) (resid 156 and name CA)
      (resid 156 and name C) (resid 157 and name N) 1 -46.8 8.6 2
assign (resid 156 and name C) (resid 157 and name N)
      (resid 157 and name CA) (resid 157 and name C) 1 -65.8 20.2 2
60 assign (resid 157 and name N) (resid 157 and name CA)
      (resid 157 and name C) (resid 158 and name N) 1 -41.9 9.7 2
assign (resid 157 and name C) (resid 158 and name N)
      (resid 158 and name CA) (resid 158 and name C) 1 -65.8 20.5 2
65 assign (resid 158 and name N) (resid 158 and name CA)
      (resid 158 and name C) (resid 159 and name N) 1 -42.8 11.4 2
assign (resid 158 and name C) (resid 159 and name N)
      (resid 159 and name CA) (resid 159 and name C) 1 -65.0 21.2 2
70 assign (resid 159 and name N) (resid 159 and name CA)
      (resid 159 and name C) (resid 160 and name N) 1 -43.7 26.1 2
assign (resid 159 and name C) (resid 160 and name N)
      (resid 160 and name CA) (resid 160 and name C) 1 -66.8 16.2 2
75 assign (resid 160 and name N) (resid 160 and name CA)
      (resid 160 and name C) (resid 161 and name N) 1 -36.5 18.1 2
assign (resid 160 and name C) (resid 161 and name N)
      (resid 161 and name CA) (resid 161 and name C) 1 -85.0 26.8 2
80 assign (resid 187 and name N) (resid 187 and name CA)
      (resid 187 and name C) (resid 188 and name N) 1 -49.2 18.5 2
assign (resid 187 and name C) (resid 188 and name N)
      (resid 188 and name CA) (resid 188 and name C) 1 -58.5 18.6 2
75 assign (resid 188 and name N) (resid 188 and name CA)
      (resid 188 and name C) (resid 189 and name N) 1 -39.6 9.8 2
assign (resid 188 and name C) (resid 189 and name N)
      (resid 189 and name CA) (resid 189 and name C) 1 -68.8 15.5 2
80 assign (resid 189 and name N) (resid 189 and name CA)
      (resid 189 and name C) (resid 190 and name N) 1 -43.8 28.8 2
assign (resid 189 and name C) (resid 190 and name N)
      (resid 190 and name CA) (resid 190 and name C) 1 -62.4 12.7 2
80 assign (resid 190 and name N) (resid 190 and name CA)
      (resid 190 and name C) (resid 191 and name N) 1 -43.6 9.5 2
assign (resid 191 and name N) (resid 191 and name CA)
      (resid 191 and name C) (resid 192 and name N) 1 -43.7 11.1 2

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assign (resid 191 and name C) (resid 192 and name N)
(resid 192 and name CA) (resid 192 and name C) 1 -62.8 8.5 2
assign (resid 192 and name N) (resid 192 and name CA)
(resid 192 and name C) (resid 193 and name N) 1 -38.7 16.2 2
5 assign (resid 192 and name C) (resid 193 and name N)
(resid 193 and name CA) (resid 193 and name C) 1 -63.7 4.9 2
assign (resid 193 and name N) (resid 193 and name CA)
(resid 193 and name C) (resid 194 and name N) 1 -44.8 7.1 2
10 assign (resid 193 and name C) (resid 194 and name N)
(resid 194 and name CA) (resid 194 and name C) 1 -63.6 7.9 2
assign (resid 194 and name N) (resid 194 and name CA)
(resid 194 and name C) (resid 195 and name N) 1 -46.5 19.5 2
assign (resid 194 and name C) (resid 195 and name N)
(resid 195 and name CA) (resid 195 and name C) 1 -59.4 18.7 2
15 assign (resid 195 and name N) (resid 195 and name CA)
(resid 195 and name C) (resid 196 and name N) 1 -40.3 7.6 2
assign (resid 195 and name C) (resid 196 and name N)
(resid 196 and name CA) (resid 196 and name C) 1 -64.8 7.6 2
20 assign (resid 196 and name N) (resid 196 and name CA)
(resid 196 and name C) (resid 197 and name N) 1 -46.6 21.4 2
assign (resid 196 and name C) (resid 197 and name N)
(resid 197 and name CA) (resid 197 and name C) 1 -56.8 24.2 2
assign (resid 197 and name N) (resid 197 and name CA)
(resid 197 and name C) (resid 198 and name N) 1 -47.9 10.8 2
25 assign (resid 197 and name C) (resid 198 and name N)
(resid 198 and name CA) (resid 198 and name C) 1 -66.3 8.1 2
assign (resid 198 and name N) (resid 198 and name CA)
(resid 198 and name C) (resid 199 and name N) 1 -42.5 16.8 2
30 assign (resid 198 and name C) (resid 199 and name N)
(resid 199 and name CA) (resid 199 and name C) 1 -54.1 19.4 2
assign (resid 199 and name N) (resid 199 and name CA)
(resid 199 and name C) (resid 200 and name N) 1 -41.6 20.9 2
assign (resid 199 and name C) (resid 200 and name N)
(resid 200 and name CA) (resid 200 and name C) 1 -66.5 9.7 2
35 assign (resid 200 and name N) (resid 200 and name CA)
(resid 200 and name C) (resid 201 and name N) 1 -38.8 17.8 2
assign (resid 200 and name C) (resid 201 and name N)
(resid 201 and name CA) (resid 201 and name C) 1 -64.9 23.6 2
40 assign (resid 201 and name N) (resid 201 and name CA)
(resid 201 and name C) (resid 202 and name N) 1 -44.1 13.4 2
assign (resid 201 and name C) (resid 202 and name N)
(resid 202 and name CA) (resid 202 and name C) 1 -60.4 10.6 2
45 assign (resid 202 and name N) (resid 202 and name CA)
(resid 202 and name C) (resid 203 and name N) 1 -43.3 8.9 2
assign (resid 202 and name C) (resid 203 and name N)
(resid 203 and name CA) (resid 203 and name C) 1 -62.0 9.1 2
50 assign (resid 203 and name N) (resid 203 and name CA)
(resid 203 and name C) (resid 204 and name N) 1 -47.2 7.9 2
assign (resid 203 and name C) (resid 204 and name N)
(resid 204 and name CA) (resid 204 and name C) 1 -63.1 5.2 2
55 assign (resid 204 and name N) (resid 204 and name CA)
(resid 204 and name C) (resid 205 and name N) 1 -34.5 15.7 2
assign (resid 204 and name C) (resid 205 and name N)
(resid 205 and name CA) (resid 205 and name C) 1 -75.5 10.2 2
60 assign (resid 205 and name N) (resid 205 and name CA)
(resid 205 and name C) (resid 206 and name N) 1 -24.5 22.8 2
assign (resid 205 and name C) (resid 206 and name N)
(resid 206 and name CA) (resid 206 and name C) 1 -74.5 15.7 2
65 assign (resid 206 and name N) (resid 206 and name CA)
(resid 206 and name C) (resid 207 and name N) 1 -32.5 16.8 2
assign (resid 206 and name C) (resid 207 and name N)
(resid 207 and name CA) (resid 207 and name C) 1 -81.8 32.8 2
70 assign (resid 219 and name N) (resid 219 and name CA)
(resid 219 and name C) (resid 220 and name N) 1 167.2 4.7 2
assign (resid 219 and name C) (resid 220 and name N)
(resid 220 and name CA) (resid 220 and name C) 1 -58.5 25.6 2
75 assign (resid 220 and name N) (resid 220 and name CA)
(resid 220 and name C) (resid 221 and name N) 1 -42.0 23.0 2
assign (resid 220 and name C) (resid 221 and name N)
(resid 221 and name CA) (resid 221 and name C) 1 -60.6 14.5 2
80 assign (resid 221 and name N) (resid 221 and name CA)
(resid 221 and name C) (resid 222 and name N) 1 -44.8 15.5 2
assign (resid 221 and name C) (resid 222 and name N)
(resid 222 and name CA) (resid 222 and name C) 1 -61.7 15.3 2
75 assign (resid 222 and name N) (resid 222 and name CA)
(resid 222 and name C) (resid 223 and name N) 1 -40.9 8.9 2
assign (resid 222 and name C) (resid 223 and name N)
(resid 223 and name CA) (resid 223 and name C) 1 -64.3 8.6 2
80 assign (resid 223 and name N) (resid 223 and name CA)
(resid 223 and name C) (resid 224 and name N) 1 -42.6 17.2 2
assign (resid 223 and name C) (resid 224 and name N)
(resid 224 and name CA) (resid 224 and name C) 1 -68.1 12.4 2
assign (resid 224 and name N) (resid 224 and name CA)

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      (resid 224 and name C) (resid 225 and name N) 1 -40.9 30.3 2
assign (resid 224 and name C) (resid 225 and name N)
      (resid 225 and name CA) (resid 225 and name C) 1 -61.3 25.1 2
assign (resid 225 and name N) (resid 225 and name CA)
5  (resid 225 and name C) (resid 226 and name N) 1 -40.7 20.8 2
assign (resid 225 and name C) (resid 226 and name N)
      (resid 226 and name CA) (resid 226 and name C) 1 -90.7 31.1 2
assign (resid 240 and name N) (resid 240 and name CA)
      (resid 240 and name C) (resid 241 and name N) 1 158.2 24.5 2
10 assign (resid 240 and name C) (resid 241 and name N)
      (resid 241 and name CA) (resid 241 and name C) 1 -58.3 12.4 2
assign (resid 241 and name N) (resid 241 and name CA)
      (resid 241 and name C) (resid 242 and name N) 1 -35.4 14.3 2
15 assign (resid 241 and name C) (resid 242 and name N)
      (resid 242 and name CA) (resid 242 and name C) 1 -69.5 22.6 2
assign (resid 242 and name N) (resid 242 and name CA)
      (resid 242 and name C) (resid 243 and name N) 1 -40.7 12.7 2
assign (resid 242 and name C) (resid 243 and name N)
      (resid 243 and name CA) (resid 243 and name C) 1 -66.8 13.1 2
20 assign (resid 243 and name N) (resid 243 and name CA)
      (resid 243 and name C) (resid 244 and name N) 1 -41.0 7.8 2
assign (resid 243 and name C) (resid 244 and name N)
      (resid 244 and name CA) (resid 244 and name C) 1 -59.4 10.8 2
25 assign (resid 244 and name N) (resid 244 and name CA)
      (resid 244 and name C) (resid 245 and name N) 1 -48.2 24.1 2
assign (resid 244 and name C) (resid 245 and name N)
      (resid 245 and name CA) (resid 245 and name C) 1 -59.5 24.8 2
30 assign (resid 245 and name N) (resid 245 and name CA)
      (resid 245 and name C) (resid 246 and name N) 1 -45.0 11.6 2
assign (resid 245 and name C) (resid 246 and name N)
      (resid 246 and name CA) (resid 246 and name C) 1 -63.4 10.6 2
35 assign (resid 246 and name N) (resid 246 and name CA)
      (resid 246 and name C) (resid 247 and name N) 1 -37.0 14.7 2
assign (resid 246 and name C) (resid 247 and name N)
      (resid 247 and name CA) (resid 247 and name C) 1 -67.5 10.5 2
40 assign (resid 247 and name N) (resid 247 and name CA)
      (resid 247 and name C) (resid 248 and name N) 1 -46.9 8.1 2
assign (resid 247 and name C) (resid 248 and name N)
      (resid 248 and name CA) (resid 248 and name C) 1 -59.2 6.5 2
45 assign (resid 248 and name N) (resid 248 and name CA)
      (resid 248 and name C) (resid 249 and name N) 1 -39.5 17.1 2
assign (resid 248 and name C) (resid 249 and name N)
      (resid 249 and name CA) (resid 249 and name C) 1 -65.8 15.2 2
50 assign (resid 249 and name N) (resid 249 and name CA)
      (resid 249 and name C) (resid 250 and name N) 1 -42.4 9.3 2
assign (resid 249 and name C) (resid 250 and name N)
      (resid 250 and name CA) (resid 250 and name C) 1 -65.6 6.9 2
55 assign (resid 250 and name N) (resid 250 and name CA)
      (resid 250 and name C) (resid 251 and name N) 1 -40.7 11.6 2
assign (resid 250 and name C) (resid 251 and name N)
      (resid 251 and name CA) (resid 251 and name C) 1 -63.2 5.8 2
60 assign (resid 251 and name N) (resid 251 and name CA)
      (resid 251 and name C) (resid 252 and name N) 1 -41.6 22.1 2
assign (resid 251 and name C) (resid 252 and name N)
      (resid 252 and name CA) (resid 252 and name C) 1 -64.6 19.2 2
65 assign (resid 252 and name N) (resid 252 and name CA)
      (resid 252 and name C) (resid 253 and name N) 1 -53.5 9.7 2
assign (resid 252 and name C) (resid 253 and name N)
      (resid 253 and name CA) (resid 253 and name C) 1 -67.5 19.3 2
70 assign (resid 253 and name N) (resid 253 and name CA)
      (resid 253 and name C) (resid 254 and name N) 1 -42.2 24.7 2
assign (resid 253 and name C) (resid 254 and name N)
      (resid 254 and name CA) (resid 254 and name C) 1 -67.7 20.4 2
75 assign (resid 254 and name N) (resid 254 and name CA)
      (resid 254 and name C) (resid 255 and name N) 1 -35.2 22.1 2
assign (resid 254 and name C) (resid 255 and name N)
      (resid 255 and name CA) (resid 255 and name C) 1 -87.2 46.4 2
80 assign (resid 255 and name N) (resid 255 and name CA)
      (resid 255 and name C) (resid 256 and name N) 1 -18.2 36.7 2
assign (resid 255 and name C) (resid 256 and name N)
      (resid 256 and name CA) (resid 256 and name C) 1 -89.2 37.3 2
assign (resid 256 and name N) (resid 256 and name CA)
      (resid 256 and name C) (resid 257 and name N) 1 -47.2 24.2 2
75 assign (resid 256 and name C) (resid 257 and name N)
      (resid 257 and name CA) (resid 257 and name C) 1 -70.3 39.1 2
assign (resid 257 and name N) (resid 257 and name CA)
      (resid 257 and name C) (resid 258 and name N) 1 -37.1 43.9 2
80 assign (resid 257 and name C) (resid 258 and name N)
      (resid 258 and name CA) (resid 258 and name C) 1 -67.7 43.1 2
assign (resid 258 and name N) (resid 258 and name CA)
      (resid 258 and name C) (resid 259 and name N) 1 -49.5 24.3 2
assign (resid 258 and name C) (resid 259 and name N)
      (resid 259 and name CA) (resid 259 and name C) 1 -65.8 14.5 2

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assign (resid 259 and name N) (resid 259 and name CA)
      (resid 259 and name C) (resid 260 and name N) 1 -38.6 7.5 2
assign (resid 259 and name C) (resid 260 and name N)
      (resid 260 and name CA) (resid 260 and name C) 1 -62.2 17.8 2
5 assign (resid 260 and name N) (resid 260 and name CA)
      (resid 260 and name C) (resid 261 and name N) 1 -46.5 12.2 2
assign (resid 260 and name C) (resid 261 and name N)
      (resid 261 and name CA) (resid 261 and name C) 1 -63.0 9.0 2
10 assign (resid 261 and name N) (resid 261 and name CA)
      (resid 261 and name C) (resid 262 and name N) 1 -39.5 24.2 2
assign (resid 261 and name C) (resid 262 and name N)
      (resid 262 and name CA) (resid 262 and name C) 1 -63.4 22.1 2
assign (resid 262 and name N) (resid 262 and name CA)
      (resid 262 and name C) (resid 263 and name N) 1 -44.5 14.6 2
15 assign (resid 262 and name C) (resid 263 and name N)
      (resid 263 and name CA) (resid 263 and name C) 1 -63.2 8.7 2
assign (resid 263 and name N) (resid 263 and name CA)
      (resid 263 and name C) (resid 264 and name N) 1 -41.8 13.4 2
20 assign (resid 263 and name C) (resid 264 and name N)
      (resid 264 and name CA) (resid 264 and name C) 1 -65.5 6.7 2
assign (resid 264 and name N) (resid 264 and name CA)
      (resid 264 and name C) (resid 265 and name N) 1 -42.5 10.0 2
assign (resid 264 and name C) (resid 265 and name N)
      (resid 265 and name CA) (resid 265 and name C) 1 -64.7 16.1 2
25 assign (resid 265 and name N) (resid 265 and name CA)
      (resid 265 and name C) (resid 266 and name N) 1 -40.7 12.8 2
assign (resid 265 and name C) (resid 266 and name N)
      (resid 266 and name CA) (resid 266 and name C) 1 -61.0 9.2 2
30 assign (resid 266 and name N) (resid 266 and name CA)
      (resid 266 and name C) (resid 267 and name N) 1 -44.5 9.2 2
assign (resid 266 and name C) (resid 267 and name N)
      (resid 267 and name CA) (resid 267 and name C) 1 -65.5 8.3 2
assign (resid 267 and name N) (resid 267 and name CA)
      (resid 267 and name C) (resid 268 and name N) 1 -40.8 6.2 2
35 assign (resid 267 and name C) (resid 268 and name N)
      (resid 268 and name CA) (resid 268 and name C) 1 -59.5 11.1 2
assign (resid 268 and name N) (resid 268 and name CA)
      (resid 268 and name C) (resid 269 and name N) 1 -45.5 10.3 2
40 assign (resid 268 and name C) (resid 269 and name N)
      (resid 269 and name CA) (resid 269 and name C) 1 -64.5 6.2 2
assign (resid 269 and name N) (resid 269 and name CA)
      (resid 269 and name C) (resid 270 and name N) 1 -42.6 13.8 2
45 assign (resid 269 and name C) (resid 270 and name N)
      (resid 270 and name CA) (resid 270 and name C) 1 -67.2 7.0 2
assign (resid 270 and name N) (resid 270 and name CA)
      (resid 270 and name C) (resid 271 and name N) 1 -33.8 10.2 2
50 assign (resid 270 and name C) (resid 271 and name N)
      (resid 271 and name CA) (resid 271 and name C) 1 -69.3 15.4 2
assign (resid 271 and name N) (resid 271 and name CA)
      (resid 271 and name C) (resid 272 and name N) 1 -34.6 11.7 2
55 assign (resid 271 and name C) (resid 272 and name N)
      (resid 272 and name CA) (resid 272 and name C) 1 -81.1 19.6 2
assign (resid 272 and name N) (resid 272 and name CA)
      (resid 272 and name C) (resid 273 and name N) 1 -131.8 7.2 2
60 assign (resid 273 and name N) (resid 273 and name CA)
      (resid 273 and name C) (resid 274 and name N) 1 76.1 5.8 2
assign (resid 274 and name N) (resid 274 and name CA)
      (resid 274 and name C) (resid 275 and name N) 1 -30.6 26.0 2
65 assign (resid 274 and name C) (resid 275 and name N)
      (resid 275 and name CA) (resid 275 and name C) 1 -65.9 12.8 2
assign (resid 275 and name N) (resid 275 and name CA)
      (resid 275 and name C) (resid 276 and name N) 1 -34.8 10.0 2
70 assign (resid 275 and name C) (resid 276 and name N)
      (resid 276 and name CA) (resid 276 and name C) 1 -72.1 8.9 2
assign (resid 276 and name N) (resid 276 and name CA)
      (resid 276 and name C) (resid 277 and name N) 1 -41.2 9.4 2
75 assign (resid 276 and name C) (resid 277 and name N)
      (resid 277 and name CA) (resid 277 and name C) 1 -60.0 4.6 2
assign (resid 277 and name N) (resid 277 and name CA)
      (resid 277 and name C) (resid 278 and name N) 1 -41.8 7.5 2
80 assign (resid 277 and name C) (resid 278 and name N)
      (resid 278 and name CA) (resid 278 and name C) 1 -64.3 12.1 2
assign (resid 278 and name N) (resid 278 and name CA)
      (resid 278 and name C) (resid 279 and name N) 1 -44.2 5.4 2
assign (resid 278 and name C) (resid 279 and name N)
      (resid 279 and name CA) (resid 279 and name C) 1 -60.6 6.6 2
assign (resid 279 and name N) (resid 279 and name CA)
      (resid 279 and name C) (resid 280 and name N) 1 -42.4 10.3 2
80 assign (resid 279 and name C) (resid 280 and name N)
      (resid 280 and name CA) (resid 280 and name C) 1 -66.0 9.3 2
assign (resid 280 and name N) (resid 280 and name CA)
      (resid 280 and name C) (resid 281 and name N) 1 -41.0 6.9 2
assign (resid 280 and name C) (resid 281 and name N)

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assign (resid 281 and name CA) (resid 281 and name C) 1 -64.7 5.8 2
 assign (resid 281 and name N) (resid 281 and name CA)
 (resid 281 and name C) (resid 282 and name N) 1 -39.2 10.6 2
 5 assign (resid 281 and name C) (resid 282 and name N)
 (resid 282 and name CA) (resid 282 and name C) 1 -70.1 19.6 2
 assign (resid 303 and name N) (resid 303 and name CA)
 (resid 303 and name C) (resid 304 and name N) 1 -25.4 31.1 2
 assign (resid 303 and name C) (resid 304 and name N)
 (resid 304 and name CA) (resid 304 and name C) 1 -79.8 20.1 2
 10 assign (resid 304 and name N) (resid 304 and name CA)
 (resid 304 and name C) (resid 305 and name N) 1 -18.4 34.5 2
 assign (resid 304 and name C) (resid 305 and name N)
 (resid 305 and name CA) (resid 305 and name C) 1 -56.6 16.6 2
 15 assign (resid 305 and name N) (resid 305 and name CA)
 (resid 305 and name C) (resid 306 and name N) 1 -45.0 6.5 2
 assign (resid 305 and name C) (resid 306 and name N)
 (resid 306 and name CA) (resid 306 and name C) 1 -61.2 9.3 2
 assign (resid 306 and name N) (resid 306 and name CA)
 (resid 306 and name C) (resid 307 and name N) 1 -39.0 8.4 2
 20 assign (resid 306 and name C) (resid 307 and name N)
 (resid 307 and name CA) (resid 307 and name C) 1 -66.8 12.5 2
 assign (resid 307 and name N) (resid 307 and name CA)
 (resid 307 and name C) (resid 308 and name N) 1 -38.5 14.2 2
 25 assign (resid 307 and name C) (resid 308 and name N)
 (resid 308 and name CA) (resid 308 and name C) 1 -63.5 8.0 2
 assign (resid 308 and name N) (resid 308 and name CA)
 (resid 308 and name C) (resid 309 and name N) 1 -45.0 12.3 2
 assign (resid 308 and name C) (resid 309 and name N)
 (resid 309 and name CA) (resid 309 and name C) 1 -61.5 9.0 2
 30 assign (resid 309 and name N) (resid 309 and name CA)
 (resid 309 and name C) (resid 310 and name N) 1 -43.0 8.0 2
 assign (resid 309 and name C) (resid 310 and name N)
 (resid 310 and name CA) (resid 310 and name C) 1 -62.1 4.4 2
 35 assign (resid 310 and name N) (resid 310 and name CA)
 (resid 310 and name C) (resid 311 and name N) 1 -42.6 11.1 2
 assign (resid 310 and name C) (resid 311 and name N)
 (resid 311 and name CA) (resid 311 and name C) 1 -67.5 12.2 2
 assign (resid 311 and name N) (resid 311 and name CA)
 (resid 311 and name C) (resid 312 and name N) 1 -35.6 11.7 2
 40 assign (resid 311 and name C) (resid 312 and name N)
 (resid 312 and name CA) (resid 312 and name C) 1 -64.7 8.9 2
 assign (resid 312 and name N) (resid 312 and name CA)
 (resid 312 and name C) (resid 313 and name N) 1 -41.8 10.0 2
 45 assign (resid 312 and name C) (resid 313 and name N)
 (resid 313 and name CA) (resid 313 and name C) 1 -68.7 6.3 2
 assign (resid 313 and name N) (resid 313 and name CA)
 (resid 313 and name C) (resid 314 and name N) 1 -32.1 15.5 2
 assign (resid 313 and name C) (resid 314 and name N)
 (resid 314 and name CA) (resid 314 and name C) 1 -69.8 18.5 2
 50 assign (resid 314 and name N) (resid 314 and name CA)
 (resid 314 and name C) (resid 315 and name N) 1 -51.9 8.1 2
 assign (resid 314 and name C) (resid 315 and name N)
 (resid 315 and name CA) (resid 315 and name C) 1 -65.1 7.9 2
 55 assign (resid 315 and name N) (resid 315 and name CA)
 (resid 315 and name C) (resid 316 and name N) 1 -44.9 14.6 2
 assign (resid 315 and name C) (resid 316 and name N)
 (resid 316 and name CA) (resid 316 and name C) 1 -105.3 52.3 2
 assign (resid 317 and name N) (resid 317 and name CA)
 (resid 317 and name C) (resid 318 and name N) 1 101.2 65.8 2
 60 assign (resid 317 and name C) (resid 318 and name N)
 (resid 318 and name CA) (resid 318 and name C) 1 -76.7 62.1 2
 assign (resid 318 and name N) (resid 318 and name CA)
 (resid 318 and name C) (resid 319 and name N) 1 -24.3 35.9 2
 65 assign (resid 318 and name C) (resid 319 and name N)
 (resid 319 and name CA) (resid 319 and name C) 1 -107.6 35.3 2
 assign (resid 322 and name C) (resid 323 and name N)
 (resid 323 and name CA) (resid 323 and name C) 1 -136.3 22.8 2
 assign (resid 323 and name N) (resid 323 and name CA)
 (resid 323 and name C) (resid 324 and name N) 1 161.3 20.8 2
 70 assign (resid 323 and name C) (resid 324 and name N)
 (resid 324 and name CA) (resid 324 and name C) 1 -129.5 25.9 2
 assign (resid 324 and name N) (resid 324 and name CA)
 (resid 324 and name C) (resid 325 and name N) 1 134.1 13.8 2
 75 assign (resid 324 and name C) (resid 325 and name N)
 (resid 325 and name CA) (resid 325 and name C) 1 -73.1 10.4 2
 assign (resid 325 and name N) (resid 325 and name CA)
 (resid 325 and name C) (resid 326 and name N) 1 126.5 32.0 2
 assign (resid 325 and name C) (resid 326 and name N)
 (resid 326 and name CA) (resid 326 and name C) 1 -83.2 28.8 2
 80 assign (resid 326 and name N) (resid 326 and name CA)
 (resid 326 and name C) (resid 327 and name N) 1 -10.0 58.2 2
 assign (resid 327 and name C) (resid 328 and name N)
 (resid 328 and name CA) (resid 328 and name C) 1 -69.5 30.5 2

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assign (resid 328 and name N) (resid 328 and name CA)
      (resid 328 and name C) (resid 329 and name N) 1 141.1 20.7 2
assign (resid 328 and name C) (resid 329 and name N)
      (resid 329 and name CA) (resid 329 and name C) 1 -151.4 21.0 2
5 assign (resid 329 and name N) (resid 329 and name CA)
      (resid 329 and name C) (resid 330 and name N) 1 148.8 37.8 2
assign (resid 329 and name C) (resid 330 and name N)
      (resid 330 and name CA) (resid 330 and name C) 1 -111.8 27.8 2
10 assign (resid 330 and name N) (resid 330 and name CA)
      (resid 330 and name C) (resid 331 and name N) 1 114.5 48.0 2
assign (resid 330 and name C) (resid 331 and name N)
      (resid 331 and name CA) (resid 331 and name C) 1 -110.6 50.3 2
assign (resid 331 and name N) (resid 331 and name CA)
      (resid 331 and name C) (resid 332 and name N) 1 120.6 15.1 2
15 assign (resid 336 and name N) (resid 336 and name CA)
      (resid 336 and name C) (resid 337 and name N) 1 111.2 24.3 2
assign (resid 336 and name C) (resid 337 and name N)
      (resid 337 and name CA) (resid 337 and name C) 1 -99.9 34.9 2
20 assign (resid 337 and name N) (resid 337 and name CA)
      (resid 337 and name C) (resid 338 and name N) 1 127.3 25.8 2
assign (resid 338 and name N) (resid 338 and name CA)
      (resid 338 and name C) (resid 339 and name N) 1 151.2 10.8 2
assign (resid 338 and name C) (resid 339 and name N)
      (resid 339 and name CA) (resid 339 and name C) 1 -52.6 14.9 2
25 assign (resid 339 and name N) (resid 339 and name CA)
      (resid 339 and name C) (resid 340 and name N) 1 135.7 16.7 2
assign (resid 339 and name C) (resid 340 and name N)
      (resid 340 and name CA) (resid 340 and name C) 1 85.6 22.0 2
30 assign (resid 340 and name N) (resid 340 and name CA)
      (resid 340 and name C) (resid 341 and name N) 1 0.6 25.8 2
assign (resid 340 and name C) (resid 341 and name N)
      (resid 341 and name CA) (resid 341 and name C) 1 -76.5 26.5 2
assign (resid 341 and name N) (resid 341 and name CA)
      (resid 341 and name C) (resid 342 and name N) 1 143.9 13.8 2
35 assign (resid 341 and name C) (resid 342 and name N)
      (resid 342 and name CA) (resid 342 and name C) 1 -92.1 13.9 2
assign (resid 342 and name N) (resid 342 and name CA)
      (resid 342 and name C) (resid 343 and name N) 1 138.2 17.9 2
40 assign (resid 342 and name C) (resid 343 and name N)
      (resid 343 and name CA) (resid 343 and name C) 1 -125.2 18.8 2
assign (resid 343 and name N) (resid 343 and name CA)
      (resid 343 and name C) (resid 344 and name N) 1 134.2 7.4 2
45 assign (resid 343 and name C) (resid 344 and name N)
      (resid 344 and name CA) (resid 344 and name C) 1 -110.5 34.5 2
assign (resid 344 and name N) (resid 344 and name CA)
      (resid 344 and name C) (resid 345 and name N) 1 121.6 16.5 2
50 assign (resid 344 and name C) (resid 345 and name N)
      (resid 345 and name CA) (resid 345 and name C) 1 -100.0 29.5 2
assign (resid 345 and name N) (resid 345 and name CA)
      (resid 345 and name C) (resid 346 and name N) 1 110.4 28.2 2
55 assign (resid 346 and name N) (resid 346 and name CA)
      (resid 346 and name C) (resid 347 and name N) 1 94.2 20.3 2
assign (resid 346 and name C) (resid 347 and name N)
      (resid 347 and name CA) (resid 347 and name C) 1 -60.2 16.7 2
60 assign (resid 347 and name N) (resid 347 and name CA)
      (resid 347 and name C) (resid 348 and name N) 1 -37.2 15.0 2
assign (resid 347 and name C) (resid 348 and name N)
      (resid 348 and name CA) (resid 348 and name C) 1 -58.5 16.0 2
65 assign (resid 348 and name N) (resid 348 and name CA)
      (resid 348 and name C) (resid 349 and name N) 1 -40.9 13.5 2
assign (resid 348 and name C) (resid 349 and name N)
      (resid 349 and name CA) (resid 349 and name C) 1 -68.0 13.2 2
70 assign (resid 349 and name N) (resid 349 and name CA)
      (resid 349 and name C) (resid 350 and name N) 1 -37.5 14.1 2
assign (resid 349 and name C) (resid 350 and name N)
      (resid 350 and name CA) (resid 350 and name C) 1 -62.5 22.2 2
75 assign (resid 350 and name N) (resid 350 and name CA)
      (resid 350 and name C) (resid 351 and name N) 1 -42.5 10.2 2
assign (resid 350 and name C) (resid 351 and name N)
      (resid 351 and name CA) (resid 351 and name C) 1 -70.3 13.1 2
80 assign (resid 351 and name N) (resid 351 and name CA)
      (resid 351 and name C) (resid 352 and name N) 1 -11.3 20.8 2
assign (resid 351 and name C) (resid 352 and name N)
      (resid 352 and name CA) (resid 352 and name C) 1 -112.3 26.1 2
75 assign (resid 352 and name N) (resid 352 and name CA)
      (resid 352 and name C) (resid 353 and name N) 1 15.4 24.8 2
assign (resid 352 and name C) (resid 353 and name N)
      (resid 353 and name CA) (resid 353 and name C) 1 -72.5 12.9 2
80 assign (resid 353 and name N) (resid 353 and name CA)
      (resid 353 and name C) (resid 354 and name N) 1 118.2 15.6 2
assign (resid 354 and name N) (resid 354 and name CA)
      (resid 354 and name C) (resid 355 and name N) 1 -26.2 19.5 2
assign (resid 354 and name C) (resid 355 and name N)

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      (resid 355 and name CA) (resid 355 and name C) 1 -72.7 19.1 2
assign (resid 355 and name N) (resid 355 and name CA)
      (resid 355 and name C) (resid 356 and name N) 1 -20.6 14.4 2
5 assign (resid 355 and name C) (resid 356 and name N)
      (resid 356 and name CA) (resid 356 and name C) 1 -104.2 27.9 2
assign (resid 356 and name N) (resid 356 and name CA)
      (resid 356 and name C) (resid 357 and name N) 1 -40.6 11.1 2
assign (resid 356 and name C) (resid 357 and name N)
      (resid 357 and name CA) (resid 357 and name C) 1 -120.1 29.1 2
10 assign (resid 359 and name N) (resid 359 and name CA)
      (resid 359 and name C) (resid 360 and name N) 1 59.7 29.3 2
assign (resid 360 and name N) (resid 360 and name CA)
      (resid 360 and name C) (resid 361 and name N) 1 -27.1 9.8 2
15 assign (resid 360 and name C) (resid 361 and name N)
      (resid 361 and name CA) (resid 361 and name C) 1 -85.0 6.2 2
assign (resid 361 and name N) (resid 361 and name CA)
      (resid 361 and name C) (resid 362 and name N) 1 -0.2 18.5 2
assign (resid 361 and name C) (resid 362 and name N)
      (resid 362 and name CA) (resid 362 and name C) 1 -97.2 22.8 2
20 assign (resid 362 and name N) (resid 362 and name CA)
      (resid 362 and name C) (resid 363 and name N) 1 133.9 18.7 2
assign (resid 362 and name C) (resid 363 and name N)
      (resid 363 and name CA) (resid 363 and name C) 1 -84.4 10.2 2
25 assign (resid 363 and name N) (resid 363 and name CA)
      (resid 363 and name C) (resid 364 and name N) 1 111.4 17.2 2
assign (resid 363 and name C) (resid 364 and name N)
      (resid 364 and name CA) (resid 364 and name C) 1 -137.7 21.3 2
30 assign (resid 364 and name N) (resid 364 and name CA)
      (resid 364 and name C) (resid 365 and name N) 1 105.5 13.3 2
assign (resid 381 and name N) (resid 381 and name CA)
      (resid 381 and name C) (resid 382 and name N) 1 136.9 66.1 2
35 assign (resid 381 and name C) (resid 382 and name N)
      (resid 382 and name CA) (resid 382 and name C) 1 -116.0 23.4 2
assign (resid 382 and name N) (resid 382 and name CA)
      (resid 382 and name C) (resid 383 and name N) 1 36.7 22.3 2
40 assign (resid 383 and name N) (resid 383 and name CA)
      (resid 383 and name C) (resid 384 and name N) 1 -25.9 12.7 2
assign (resid 383 and name C) (resid 384 and name N)
      (resid 384 and name CA) (resid 384 and name C) 1 -101.8 9.6 2
45 assign (resid 384 and name N) (resid 384 and name CA)
      (resid 384 and name C) (resid 385 and name N) 1 13.2 7.6 2
assign (resid 384 and name C) (resid 385 and name N)
      (resid 385 and name CA) (resid 385 and name C) 1 88.0 17.8 2
50 assign (resid 385 and name N) (resid 385 and name CA)
      (resid 385 and name C) (resid 386 and name N) 1 -162.2 7.6 2
assign (resid 385 and name C) (resid 386 and name N)
      (resid 386 and name CA) (resid 386 and name C) 1 -161.4 26.5 2
55 assign (resid 388 and name N) (resid 388 and name CA)
      (resid 388 and name C) (resid 389 and name N) 1 -21.9 29.0 2
assign (resid 388 and name C) (resid 389 and name N)
      (resid 389 and name CA) (resid 389 and name C) 1 -97.9 18.5 2
60 assign (resid 389 and name N) (resid 389 and name CA)
      (resid 389 and name C) (resid 390 and name N) 1 17.1 14.3 2
assign (resid 389 and name C) (resid 390 and name N)
      (resid 390 and name CA) (resid 390 and name C) 1 -57.7 23.2 2
65 assign (resid 390 and name N) (resid 391 and name N)
      (resid 391 and name CA) (resid 391 and name C) 1 -51.5 25.2 2
assign (resid 391 and name N) (resid 391 and name CA)
      (resid 391 and name C) (resid 392 and name N) 1 124.0 28.1 2
70 assign (resid 391 and name C) (resid 392 and name N)
      (resid 392 and name CA) (resid 392 and name C) 1 -73.3 31.9 2
assign (resid 392 and name N) (resid 392 and name CA)
      (resid 392 and name C) (resid 393 and name N) 1 -30.5 12.2 2
75 assign (resid 392 and name C) (resid 393 and name N)
      (resid 393 and name CA) (resid 393 and name C) 1 -88.5 17.4 2
assign (resid 393 and name N) (resid 393 and name CA)
      (resid 393 and name C) (resid 394 and name N) 1 9.1 21.0 2
80 assign (resid 393 and name C) (resid 394 and name N)
      (resid 394 and name CA) (resid 394 and name C) 1 -49.1 23.6 2
assign (resid 394 and name N) (resid 394 and name CA)
      (resid 394 and name C) (resid 395 and name N) 1 -44.5 17.2 2
assign (resid 394 and name C) (resid 395 and name N)
      (resid 395 and name CA) (resid 395 and name C) 1 -66.5 22.1 2
75 assign (resid 395 and name N) (resid 395 and name CA)
      (resid 395 and name C) (resid 396 and name N) 1 -45.3 25.9 2
assign (resid 395 and name C) (resid 396 and name N)
      (resid 396 and name CA) (resid 396 and name C) 1 -65.0 6.8 2
80 assign (resid 396 and name N) (resid 396 and name CA)
      (resid 396 and name C) (resid 397 and name N) 1 -41.9 18.4 2
assign (resid 396 and name C) (resid 397 and name N)
      (resid 397 and name CA) (resid 397 and name C) 1 -61.9 6.6 2
assign (resid 397 and name N) (resid 397 and name CA)
      (resid 397 and name C) (resid 398 and name N) 1 -44.5 6.8 2

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assign (resid 397 and name C) (resid 398 and name N)
(resid 398 and name CA) (resid 398 and name C) 1 -67.7 12.6 2
assign (resid 398 and name N) (resid 398 and name CA)
(resid 398 and name C) (resid 399 and name N) 1 -35.5 8.6 2
5 assign (resid 398 and name C) (resid 399 and name N)
(resid 399 and name CA) (resid 399 and name C) 1 -66.8 7.6 2
assign (resid 399 and name N) (resid 399 and name CA)
(resid 399 and name C) (resid 400 and name N) 1 -48.7 17.9 2
10 assign (resid 399 and name C) (resid 400 and name N)
(resid 400 and name CA) (resid 400 and name C) 1 -59.0 23.0 2
assign (resid 400 and name N) (resid 400 and name CA)
(resid 400 and name C) (resid 401 and name N) 1 -44.0 17.1 2
assign (resid 400 and name C) (resid 401 and name N)
(resid 401 and name CA) (resid 401 and name C) 1 -64.9 9.8 2
15 assign (resid 401 and name N) (resid 401 and name CA)
(resid 401 and name C) (resid 402 and name N) 1 -45.3 13.0 2
assign (resid 401 and name C) (resid 402 and name N)
(resid 402 and name CA) (resid 402 and name C) 1 -64.7 3.5 2
20 assign (resid 402 and name N) (resid 402 and name CA)
(resid 402 and name C) (resid 403 and name N) 1 -43.7 11.9 2
assign (resid 402 and name C) (resid 403 and name N)
(resid 403 and name CA) (resid 403 and name C) 1 -64.3 8.6 2
assign (resid 403 and name N) (resid 403 and name CA)
(resid 403 and name C) (resid 404 and name N) 1 -45.6 13.2 2
25 assign (resid 403 and name C) (resid 404 and name N)
(resid 404 and name CA) (resid 404 and name C) 1 -62.2 8.8 2
assign (resid 404 and name N) (resid 404 and name CA)
(resid 404 and name C) (resid 405 and name N) 1 -52.6 11.4 2
30 assign (resid 404 and name C) (resid 405 and name N)
(resid 405 and name CA) (resid 405 and name C) 1 -63.6 20.1 2
assign (resid 405 and name N) (resid 405 and name CA)
(resid 405 and name C) (resid 406 and name N) 1 -38.7 34.2 2
assign (resid 405 and name C) (resid 406 and name N)
(resid 406 and name CA) (resid 406 and name C) 1 -66.3 35.2 2
35 assign (resid 406 and name N) (resid 406 and name CA)
(resid 406 and name C) (resid 407 and name N) 1 -38.5 34.2 2
assign (resid 406 and name C) (resid 407 and name N)
(resid 407 and name CA) (resid 407 and name C) 1 -78.4 39.5 2
40 assign (resid 407 and name N) (resid 407 and name CA)
(resid 407 and name C) (resid 408 and name N) 1 -37.4 12.5 2
assign (resid 407 and name C) (resid 408 and name N)
(resid 408 and name CA) (resid 408 and name C) 1 -63.6 21.4 2
45 assign (resid 408 and name N) (resid 408 and name CA)
(resid 408 and name C) (resid 409 and name N) 1 -49.5 14.2 2
assign (resid 408 and name C) (resid 409 and name N)
(resid 409 and name CA) (resid 409 and name C) 1 -70.7 18.9 2
50 assign (resid 409 and name N) (resid 409 and name CA)
(resid 409 and name C) (resid 410 and name N) 1 -22.7 23.0 2
assign (resid 409 and name C) (resid 410 and name N)
(resid 410 and name CA) (resid 410 and name C) 1 -75.5 17.4 2
55 assign (resid 410 and name N) (resid 410 and name CA)
(resid 410 and name C) (resid 411 and name N) 1 -31.8 21.4 2
assign (resid 410 and name C) (resid 411 and name N)
(resid 411 and name CA) (resid 411 and name C) 1 -91.0 20.8 2
60 assign (resid 411 and name N) (resid 411 and name CA)
(resid 411 and name C) (resid 412 and name N) 1 -25.1 25.1 2
assign (resid 411 and name C) (resid 412 and name N)
(resid 412 and name CA) (resid 412 and name C) 1 -128.2 19.9 2
65 assign (resid 413 and name C) (resid 414 and name N)
(resid 414 and name CA) (resid 414 and name C) 1 -104.5 73.7 2
assign (resid 414 and name N) (resid 414 and name CA)
(resid 414 and name C) (resid 415 and name N) 1 140.1 33.5 2
70 assign (resid 414 and name C) (resid 415 and name N)
(resid 415 and name CA) (resid 415 and name C) 1 -128.6 53.1 2
assign (resid 415 and name N) (resid 415 and name CA)
(resid 415 and name C) (resid 416 and name N) 1 146.6 27.0 2
75 assign (resid 416 and name C) (resid 417 and name N)
(resid 417 and name CA) (resid 417 and name C) 1 -86.5 53.5 2
assign (resid 423 and name C) (resid 424 and name N)
(resid 424 and name CA) (resid 424 and name C) 1 -85.3 52.2 2
80 assign (resid 424 and name N) (resid 424 and name CA)
(resid 424 and name C) (resid 425 and name N) 1 109.9 87.6 2
assign (resid 424 and name C) (resid 425 and name N)
(resid 425 and name CA) (resid 425 and name C) 1 -82.5 38.2 2
assign (resid 425 and name N) (resid 425 and name CA)
(resid 425 and name C) (resid 426 and name N) 1 118.3 30.0 2
assign (resid 425 and name C) (resid 426 and name N)
(resid 426 and name CA) (resid 426 and name C) 1 -99.7 34.0 2
assign (resid 426 and name N) (resid 426 and name CA)
(resid 426 and name C) (resid 427 and name N) 1 143.5 27.8 2
assign (resid 426 and name C) (resid 427 and name N)
(resid 427 and name CA) (resid 427 and name C) 1 -86.8 39.9 2
assign (resid 427 and name N) (resid 427 and name CA)

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    assign (resid 427 and name C) (resid 428 and name N) 1 140.6 30.4 2
    assign (resid 427 and name C) (resid 428 and name N)
    assign (resid 428 and name CA) (resid 428 and name C) 1 -92.3 48.9 2
5    assign (resid 428 and name N) (resid 428 and name CA)
    assign (resid 428 and name C) (resid 429 and name N) 1 109.3 58.1 2
    assign (resid 428 and name C) (resid 429 and name N)
    assign (resid 429 and name CA) (resid 429 and name C) 1 -101.7 82.7 2
    assign (resid 430 and name C) (resid 431 and name N)
    assign (resid 431 and name CA) (resid 431 and name C) 1 -87.9 43.1 2
10   assign (resid 434 and name C) (resid 435 and name N)
    assign (resid 435 and name CA) (resid 435 and name C) 1 -95.0 58.0 2
    assign (resid 435 and name N) (resid 435 and name CA)
    assign (resid 435 and name C) (resid 436 and name N) 1 132.4 36.3 2
    assign (resid 435 and name C) (resid 436 and name N)
15   assign (resid 436 and name CA) (resid 436 and name C) 1 -79.4 30.0 2
    assign (resid 437 and name C) (resid 438 and name N)
    assign (resid 438 and name CA) (resid 438 and name C) 1 -128.8 49.4 2
    assign (resid 438 and name N) (resid 438 and name CA)
    assign (resid 438 and name C) (resid 439 and name N) 1 108.3 49.2 2
20   assign (resid 438 and name C) (resid 439 and name N)
    assign (resid 439 and name CA) (resid 439 and name C) 1 -89.2 49.8 2
    assign (resid 439 and name N) (resid 439 and name CA)
    assign (resid 439 and name C) (resid 440 and name N) 1 132.3 28.1 2
    assign (resid 439 and name C) (resid 440 and name N)
25   assign (resid 440 and name CA) (resid 440 and name C) 1 -133.3 31.6 2
    assign (resid 6 and name N) (resid 6 and name CA)
    assign (resid 6 and name CB) (resid 6 and name CG) 1 -60.0 60.0 2
    assign (resid 7 and name N) (resid 7 and name CA)
    assign (resid 7 and name CB) (resid 7 and name SG) 1 -60.0 60.0 2
30   assign (resid 8 and name N) (resid 8 and name CA)
    assign (resid 8 and name CB) (resid 8 and name CG) 1 -60.0 60.0 2
    assign (resid 8 and name CA) (resid 8 and name CB)
    assign (resid 8 and name CG) (resid 8 and name SD) 1 180.0 60.0 2
    assign (resid 9 and name N) (resid 9 and name CA)
35   assign (resid 9 and name CB) (resid 9 and name CG) 1 180.0 60.0 2
    assign (resid 9 and name CA) (resid 9 and name CB)
    assign (resid 9 and name CG) (resid 9 and name CD1) 1 90.0 30.0 2
    assign (resid 10 and name N) (resid 10 and name CA)
    assign (resid 10 and name CB) (resid 10 and name CG) 1 -60.0 60.0 2
40   assign (resid 10 and name CA) (resid 10 and name CB)
    assign (resid 10 and name CG) (resid 10 and name OD1) 1 -60.0 60.0 2
    assign (resid 11 and name N) (resid 11 and name CA)
    assign (resid 11 and name CB) (resid 11 and name CG) 1 -60.0 60.0 2
    assign (resid 11 and name CA) (resid 11 and name CB)
45   assign (resid 11 and name CG) (resid 11 and name SD) 1 180.0 60.0 2
    assign (resid 12 and name N) (resid 12 and name CA)
    assign (resid 12 and name CB) (resid 12 and name CG) 1 -60.0 60.0 2
    assign (resid 12 and name CA) (resid 12 and name CB)
    assign (resid 12 and name CG) (resid 12 and name CD) 1 180.0 60.0 2
50   assign (resid 19 and name N) (resid 19 and name CA)
    assign (resid 19 and name CB) (resid 19 and name CG) 1 -60.0 60.0 2
    assign (resid 19 and name CA) (resid 19 and name CB)
    assign (resid 19 and name CG) (resid 19 and name CD) 1 180.0 60.0 2
55   assign (resid 33 and name N) (resid 33 and name CA)
    assign (resid 33 and name CB) (resid 33 and name CG1) 1 -60.0 60.0 2
    assign (resid 34 and name N) (resid 34 and name CA)
    assign (resid 34 and name CB) (resid 34 and name OG1) 1 60.0 60.0 2
    assign (resid 37 and name N) (resid 37 and name CA)
    assign (resid 37 and name CB) (resid 37 and name CG) 1 -60.0 60.0 2
60   assign (resid 37 and name CA) (resid 37 and name CB)
    assign (resid 37 and name CG) (resid 37 and name OD1) 1 0.0 30.0 2
    assign (resid 38 and name N) (resid 38 and name CA)
    assign (resid 38 and name CB) (resid 38 and name CG) 1 -60.0 60.0 2
    assign (resid 38 and name CA) (resid 38 and name CB)
65   assign (resid 38 and name CG) (resid 38 and name SD) 1 180.0 60.0 2
    assign (resid 39 and name N) (resid 39 and name CA)
    assign (resid 39 and name CB) (resid 39 and name CG1) 1 -60.0 60.0 2
    assign (resid 40 and name N) (resid 40 and name CA)
    assign (resid 40 and name CB) (resid 40 and name CG) 1 180.0 60.0 2
70   assign (resid 40 and name CA) (resid 40 and name CB)
    assign (resid 40 and name CG) (resid 40 and name CD) 1 180.0 60.0 2
    assign (resid 41 and name N) (resid 41 and name CA)
    assign (resid 41 and name CB) (resid 41 and name OG1) 1 -60.0 60.0 2
    assign (resid 68 and name N) (resid 68 and name CA)
75   assign (resid 68 and name CB) (resid 68 and name OG) 1 60.0 60.0 2
    assign (resid 71 and name N) (resid 71 and name CA)
    assign (resid 71 and name CB) (resid 71 and name CG) 1 -60.0 60.0 2
    assign (resid 74 and name N) (resid 74 and name CA)
    assign (resid 74 and name CB) (resid 74 and name CG) 1 -60.0 60.0 2
80   assign (resid 74 and name CA) (resid 74 and name CB)
    assign (resid 74 and name CG) (resid 74 and name CD) 1 180.0 60.0 2
    assign (resid 75 and name N) (resid 75 and name CA)
    assign (resid 75 and name CB) (resid 75 and name CG) 1 180.0 60.0 2

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assign (resid 77 and name N) (resid 77 and name CA)
(resid 77 and name CB) (resid 77 and name CG) 1 -60.0 60.0 2
assign (resid 77 and name CA) (resid 77 and name CB)
(resid 77 and name CG) (resid 77 and name CD) 1 180.0 60.0 2
5 assign (resid 78 and name N) (resid 78 and name CA)
(resid 78 and name CB) (resid 78 and name CG) 1 -60.0 60.0 2
assign (resid 78 and name CA) (resid 78 and name CB)
(resid 78 and name CG) (resid 78 and name CD1) 1 180.0 60.0 2
10 assign (resid 79 and name N) (resid 79 and name CA)
(resid 79 and name CB) (resid 79 and name CG) 1 180.0 60.0 2
assign (resid 79 and name CA) (resid 79 and name CB)
(resid 79 and name CG) (resid 79 and name CD) 1 180.0 60.0 2
assign (resid 80 and name N) (resid 80 and name CA)
(resid 80 and name CB) (resid 80 and name OG) 1 -60.0 60.0 2
15 assign (resid 81 and name N) (resid 81 and name CA)
(resid 81 and name CB) (resid 81 and name CG) 1 -60.0 60.0 2
assign (resid 81 and name CA) (resid 81 and name CB)
(resid 81 and name CG) (resid 81 and name CD1) 1 180.0 60.0 2
20 assign (resid 82 and name N) (resid 82 and name CA)
(resid 82 and name CB) (resid 82 and name CG) 1 -60.0 60.0 2
assign (resid 82 and name CA) (resid 82 and name CB)
(resid 82 and name CG) (resid 82 and name CD1) 1 180.0 60.0 2
assign (resid 83 and name N) (resid 83 and name CA)
(resid 83 and name CB) (resid 83 and name OG) 1 60.0 60.0 2
25 assign (resid 85 and name N) (resid 85 and name CA)
(resid 85 and name CB) (resid 85 and name OG1) 1 60.0 60.0 2
assign (resid 86 and name N) (resid 86 and name CA)
(resid 86 and name CB) (resid 86 and name CG) 1 -60.0 60.0 2
30 assign (resid 86 and name CA) (resid 86 and name CB)
(resid 86 and name CG) (resid 86 and name CD1) 1 90.0 30.0 2
assign (resid 94 and name N) (resid 94 and name CA)
(resid 94 and name CB) (resid 94 and name CG) 1 -60.0 60.0 2
assign (resid 95 and name N) (resid 95 and name CA)
(resid 95 and name CB) (resid 95 and name CG1) 1 180.0 60.0 2
35 assign (resid 97 and name N) (resid 97 and name CA)
(resid 97 and name CB) (resid 97 and name CG1) 1 -60.0 60.0 2
assign (resid 98 and name N) (resid 98 and name CA)
(resid 98 and name CB) (resid 98 and name CG1) 1 -60.0 60.0 2
40 assign (resid 100 and name N) (resid 100 and name CA)
(resid 100 and name CB) (resid 100 and name CG) 1 -60.0 60.0 2
assign (resid 100 and name CA) (resid 100 and name CB)
(resid 100 and name CG) (resid 100 and name CD) 1 180.0 60.0 2
assign (resid 101 and name N) (resid 101 and name CA)
(resid 101 and name CB) (resid 101 and name CG) 1 180.0 60.0 2
45 assign (resid 101 and name CA) (resid 101 and name CB)
(resid 101 and name CG) (resid 101 and name CD1) 1 90.0 30.0 2
assign (resid 103 and name N) (resid 103 and name CA)
(resid 103 and name CB) (resid 103 and name CG) 1 -60.0 60.0 2
50 assign (resid 103 and name CA) (resid 103 and name CB)
(resid 103 and name CG) (resid 103 and name OD1) 1 0.0 30.0 2
assign (resid 104 and name N) (resid 104 and name CA)
(resid 104 and name CB) (resid 104 and name CG1) 1 180.0 60.0 2
55 assign (resid 105 and name N) (resid 105 and name CA)
(resid 105 and name CB) (resid 105 and name CG) 1 -60.0 60.0 2
assign (resid 105 and name CA) (resid 105 and name CB)
(resid 105 and name CG) (resid 105 and name CD1) 1 180.0 60.0 2
60 assign (resid 106 and name N) (resid 106 and name CA)
(resid 106 and name CB) (resid 106 and name CG1) 1 180.0 60.0 2
assign (resid 108 and name N) (resid 108 and name CA)
(resid 108 and name CB) (resid 108 and name CG) 1 -60.0 60.0 2
65 assign (resid 108 and name CA) (resid 108 and name CB)
(resid 108 and name CG) (resid 108 and name OD1) 1 0.0 30.0 2
assign (resid 109 and name N) (resid 109 and name CA)
(resid 109 and name CB) (resid 109 and name CG) 1 -60.0 60.0 2
70 assign (resid 109 and name CA) (resid 109 and name CB)
(resid 109 and name CG) (resid 109 and name CD1) 1 180.0 60.0 2
assign (resid 110 and name N) (resid 110 and name CA)
(resid 110 and name CB) (resid 110 and name CG) 1 -60.0 60.0 2
75 assign (resid 110 and name CA) (resid 110 and name CB)
(resid 110 and name CG) (resid 110 and name CD) 1 180.0 60.0 2
assign (resid 111 and name N) (resid 111 and name CA)
(resid 111 and name CB) (resid 111 and name CG) 1 -60.0 60.0 2
80 assign (resid 111 and name CA) (resid 111 and name CB)
(resid 111 and name CG) (resid 111 and name CD) 1 180.0 60.0 2
assign (resid 120 and name N) (resid 120 and name CA)
(resid 120 and name CB) (resid 120 and name OG1) 1 -60.0 60.0 2
assign (resid 121 and name N) (resid 121 and name CA)
(resid 121 and name CB) (resid 121 and name CG) 1 -60.0 60.0 2
assign (resid 121 and name CA) (resid 121 and name CB)
(resid 121 and name CG) (resid 121 and name CD1) 1 180.0 60.0 2
assign (resid 124 and name N) (resid 124 and name CA)
(resid 124 and name CB) (resid 124 and name CG1) 1 180.0 60.0 2
assign (resid 128 and name N) (resid 128 and name CA)

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      (resid 128 and name CB) (resid 128 and name CG) 1 180.0 60.0 2
assign (resid 128 and name CA) (resid 128 and name CB)
      (resid 128 and name CG) (resid 128 and name CD1) 1 90.0 30.0 2
5 assign (resid 130 and name N) (resid 130 and name CA)
      (resid 130 and name CB) (resid 130 and name CG) 1 -60.0 60.0 2
assign (resid 130 and name CA) (resid 130 and name CB)
      (resid 130 and name CG) (resid 130 and name SD) 1 180.0 60.0 2
assign (resid 131 and name N) (resid 131 and name CA)
      (resid 131 and name CB) (resid 131 and name CG) 1 -60.0 60.0 2
10 assign (resid 131 and name CA) (resid 131 and name CB)
      (resid 131 and name CG) (resid 131 and name OD1) 1 0.0 30.0 2
assign (resid 132 and name N) (resid 132 and name CA)
      (resid 132 and name CB) (resid 132 and name CG1) 1 180.0 60.0 2
assign (resid 133 and name N) (resid 133 and name CA)
      (resid 133 and name CB) (resid 133 and name CG1) 1 -60.0 60.0 2
15 assign (resid 135 and name N) (resid 135 and name CA)
      (resid 135 and name CB) (resid 135 and name OG) 1 -60.0 60.0 2
assign (resid 136 and name N) (resid 136 and name CA)
      (resid 136 and name CB) (resid 136 and name OG1) 1 60.0 60.0 2
20 assign (resid 138 and name N) (resid 138 and name CA)
      (resid 138 and name CB) (resid 138 and name CG) 1 -60.0 60.0 2
assign (resid 138 and name CA) (resid 138 and name CB)
      (resid 138 and name CG) (resid 138 and name CD1) 1 90.0 30.0 2
assign (resid 140 and name N) (resid 140 and name CA)
      (resid 140 and name CB) (resid 140 and name CG1) 1 180.0 60.0 2
25 assign (resid 152 and name N) (resid 152 and name CA)
      (resid 152 and name CB) (resid 152 and name CG) 1 180.0 60.0 2
assign (resid 152 and name CA) (resid 152 and name CB)
      (resid 152 and name CG) (resid 152 and name CD1) 1 90.0 30.0 2
30 assign (resid 153 and name N) (resid 153 and name CA)
      (resid 153 and name CB) (resid 153 and name CG1) 1 180.0 60.0 2
assign (resid 154 and name N) (resid 154 and name CA)
      (resid 154 and name CB) (resid 154 and name CG) 1 -60.0 60.0 2
35 assign (resid 154 and name CA) (resid 154 and name CB)
      (resid 154 and name CG) (resid 154 and name CD) 1 180.0 60.0 2
assign (resid 156 and name N) (resid 156 and name CA)
      (resid 156 and name CB) (resid 156 and name OG1) 1 -60.0 60.0 2
assign (resid 157 and name N) (resid 157 and name CA)
      (resid 157 and name CB) (resid 157 and name CG) 1 180.0 60.0 2
40 assign (resid 157 and name CA) (resid 157 and name CB)
      (resid 157 and name CG) (resid 157 and name CD) 1 180.0 60.0 2
assign (resid 158 and name N) (resid 158 and name CA)
      (resid 158 and name CB) (resid 158 and name CG) 1 180.0 60.0 2
45 assign (resid 158 and name CA) (resid 158 and name CB)
      (resid 158 and name CG) (resid 158 and name CD) 1 180.0 60.0 2
assign (resid 160 and name N) (resid 160 and name CA)
      (resid 160 and name CB) (resid 160 and name CG) 1 -60.0 60.0 2
assign (resid 160 and name CA) (resid 160 and name CB)
      (resid 160 and name CG) (resid 160 and name CD1) 1 180.0 60.0 2
50 assign (resid 188 and name N) (resid 188 and name CA)
      (resid 188 and name CB) (resid 188 and name SG) 1 -60.0 60.0 2
assign (resid 189 and name N) (resid 189 and name CA)
      (resid 189 and name CB) (resid 189 and name CG1) 1 180.0 60.0 2
55 assign (resid 190 and name N) (resid 190 and name CA)
      (resid 190 and name CB) (resid 190 and name CG) 1 180.0 60.0 2
assign (resid 190 and name CA) (resid 190 and name CB)
      (resid 190 and name CG) (resid 190 and name CD1) 1 90.0 30.0 2
assign (resid 192 and name N) (resid 192 and name CA)
      (resid 192 and name CB) (resid 192 and name CG) 1 -60.0 60.0 2
60 assign (resid 192 and name CA) (resid 192 and name CB)
      (resid 192 and name CG) (resid 192 and name CD) 1 180.0 60.0 2
assign (resid 193 and name N) (resid 193 and name CA)
      (resid 193 and name CB) (resid 193 and name CG) 1 -60.0 60.0 2
65 assign (resid 193 and name CA) (resid 193 and name CB)
      (resid 193 and name CG) (resid 193 and name CD) 1 180.0 60.0 2
assign (resid 194 and name N) (resid 194 and name CA)
      (resid 194 and name CB) (resid 194 and name CG1) 1 180.0 60.0 2
assign (resid 195 and name N) (resid 195 and name CA)
      (resid 195 and name CB) (resid 195 and name OG1) 1 -60.0 60.0 2
70 assign (resid 197 and name N) (resid 197 and name CA)
      (resid 197 and name CB) (resid 197 and name CG) 1 180.0 60.0 2
assign (resid 197 and name CA) (resid 197 and name CB)
      (resid 197 and name CG) (resid 197 and name CD1) 1 90.0 30.0 2
75 assign (resid 198 and name N) (resid 198 and name CA)
      (resid 198 and name CB) (resid 198 and name CG) 1 -60.0 60.0 2
assign (resid 198 and name CA) (resid 198 and name CB)
      (resid 198 and name CG) (resid 198 and name CD1) 1 180.0 60.0 2
assign (resid 200 and name N) (resid 200 and name CA)
      (resid 200 and name CB) (resid 200 and name CG) 1 -60.0 60.0 2
80 assign (resid 200 and name CA) (resid 200 and name CB)
      (resid 200 and name CG) (resid 200 and name CD) 1 180.0 60.0 2
assign (resid 201 and name N) (resid 201 and name CA)
      (resid 201 and name CB) (resid 201 and name OG) 1 -60.0 60.0 2

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assign (resid 202 and name N) (resid 202 and name CA)
(resid 202 and name CB) (resid 202 and name CG1) 1 180.0 60.0 2
assign (resid 203 and name N) (resid 203 and name CA)
(resid 203 and name CB) (resid 203 and name CG) 1 180.0 60.0 2
5 assign (resid 203 and name CA) (resid 203 and name CB)
(resid 203 and name CG) (resid 203 and name CD) 1 180.0 60.0 2
assign (resid 204 and name N) (resid 204 and name CA)
(resid 204 and name CB) (resid 204 and name CG) 1 -60.0 60.0 2
10 assign (resid 204 and name CA) (resid 204 and name CB)
(resid 204 and name CG) (resid 204 and name CD) 1 180.0 60.0 2
assign (resid 205 and name N) (resid 205 and name CA)
(resid 205 and name CB) (resid 205 and name CG) 1 -60.0 60.0 2
assign (resid 205 and name CA) (resid 205 and name CB)
(resid 205 and name CG) (resid 205 and name SD) 1 180.0 60.0 2
15 assign (resid 206 and name N) (resid 206 and name CA)
(resid 206 and name CB) (resid 206 and name CG) 1 -60.0 60.0 2
assign (resid 206 and name CA) (resid 206 and name CB)
(resid 206 and name CG) (resid 206 and name CD) 1 180.0 60.0 2
20 assign (resid 207 and name N) (resid 207 and name CA)
(resid 207 and name CB) (resid 207 and name CG) 1 -60.0 60.0 2
assign (resid 207 and name CA) (resid 207 and name CB)
(resid 207 and name CG) (resid 207 and name CD) 1 180.0 60.0 2
25 assign (resid 221 and name N) (resid 221 and name CA)
(resid 221 and name CB) (resid 221 and name CG) 1 -60.0 60.0 2
assign (resid 221 and name CA) (resid 221 and name CB)
(resid 221 and name CG) (resid 221 and name CD1) 1 180.0 60.0 2
30 assign (resid 222 and name N) (resid 222 and name CA)
(resid 222 and name CB) (resid 222 and name CG) 1 -60.0 60.0 2
assign (resid 222 and name CA) (resid 222 and name CB)
(resid 222 and name CG) (resid 222 and name CD) 1 180.0 60.0 2
35 assign (resid 223 and name N) (resid 223 and name CA)
(resid 223 and name CB) (resid 223 and name CG) 1 -60.0 60.0 2
assign (resid 223 and name CA) (resid 223 and name CB)
(resid 223 and name CG) (resid 223 and name CD1) 1 180.0 60.0 2
40 assign (resid 224 and name N) (resid 224 and name CA)
(resid 224 and name CB) (resid 224 and name CG) 1 -60.0 60.0 2
assign (resid 224 and name CA) (resid 224 and name CB)
(resid 224 and name CG) (resid 224 and name SD) 1 180.0 60.0 2
45 assign (resid 225 and name N) (resid 225 and name CA)
(resid 225 and name CB) (resid 225 and name CG1) 1 -60.0 60.0 2
assign (resid 241 and name N) (resid 241 and name CA)
(resid 241 and name CB) (resid 241 and name CG) 1 -60.0 60.0 2
50 assign (resid 241 and name CA) (resid 241 and name CB)
(resid 241 and name CG) (resid 241 and name OD1) 1 -60.0 60.0 2
assign (resid 242 and name N) (resid 242 and name CA)
(resid 242 and name CB) (resid 242 and name CG) 1 -60.0 60.0 2
55 assign (resid 242 and name CA) (resid 242 and name CB)
(resid 242 and name CG) (resid 242 and name CD1) 1 180.0 60.0 2
assign (resid 243 and name N) (resid 243 and name CA)
(resid 243 and name CB) (resid 243 and name CG) 1 -60.0 60.0 2
60 assign (resid 243 and name CA) (resid 243 and name CB)
(resid 243 and name CG) (resid 243 and name CD) 1 180.0 60.0 2
assign (resid 245 and name N) (resid 245 and name CA)
(resid 245 and name CB) (resid 245 and name CG1) 1 180.0 60.0 2
65 assign (resid 247 and name N) (resid 247 and name CA)
(resid 247 and name CB) (resid 247 and name CG) 1 -60.0 60.0 2
assign (resid 247 and name CA) (resid 247 and name CB)
(resid 247 and name CG) (resid 247 and name CD) 1 180.0 60.0 2
70 assign (resid 248 and name N) (resid 248 and name CA)
(resid 248 and name CB) (resid 248 and name OG) 1 60.0 60.0 2
assign (resid 249 and name N) (resid 249 and name CA)
(resid 249 and name CB) (resid 249 and name CG1) 1 -60.0 60.0 2
75 assign (resid 250 and name N) (resid 250 and name CA)
(resid 250 and name CB) (resid 250 and name CG1) 1 -60.0 60.0 2
80 assign (resid 251 and name N) (resid 251 and name CA)
(resid 251 and name CB) (resid 251 and name CG) 1 180.0 60.0 2
assign (resid 251 and name CA) (resid 251 and name CB)
(resid 251 and name CG) (resid 251 and name CD1) 1 90.0 30.0 2
70 assign (resid 252 and name N) (resid 252 and name CA)
(resid 252 and name CB) (resid 252 and name CG1) 1 -60.0 60.0 2
assign (resid 253 and name N) (resid 253 and name CA)
(resid 253 and name CB) (resid 253 and name CG) 1 180.0 60.0 2
75 assign (resid 253 and name CA) (resid 253 and name CB)
(resid 253 and name CG) (resid 253 and name CD1) 1 90.0 30.0 2
80 assign (resid 259 and name N) (resid 259 and name CA)
(resid 259 and name CB) (resid 259 and name CG1) 1 60.0 60.0 2
assign (resid 260 and name N) (resid 260 and name CA)
(resid 260 and name CB) (resid 260 and name OG) 1 -60.0 60.0 2
assign (resid 262 and name N) (resid 262 and name CA)
(resid 262 and name CB) (resid 262 and name CG1) 1 180.0 60.0 2
80 assign (resid 263 and name N) (resid 263 and name CA)
(resid 263 and name CB) (resid 263 and name CG) 1 -60.0 60.0 2
assign (resid 263 and name CA) (resid 263 and name CB)

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      (resid 263 and name CG) (resid 263 and name CD1) 1 180.0 60.0 2
assign (resid 264 and name N) (resid 264 and name CA)
      (resid 264 and name CB) (resid 264 and name OG) 1 -60.0 60.0 2
5 assign (resid 265 and name N) (resid 265 and name CA)
      (resid 265 and name CB) (resid 265 and name CG) 1 180.0 60.0 2
assign (resid 265 and name CA) (resid 265 and name CB)
      (resid 265 and name CG) (resid 265 and name CD1) 1 90.0 30.0 2
assign (resid 266 and name N) (resid 266 and name CA)
      (resid 266 and name CB) (resid 266 and name CG1) 1 -60.0 60.0 2
10 assign (resid 267 and name N) (resid 267 and name CA)
      (resid 267 and name CB) (resid 267 and name CG) 1 -60.0 60.0 2
assign (resid 267 and name CA) (resid 267 and name CB)
      (resid 267 and name CG) (resid 267 and name SD) 1 180.0 60.0 2
15 assign (resid 268 and name N) (resid 268 and name CA)
      (resid 268 and name CB) (resid 268 and name CG) 1 180.0 60.0 2
assign (resid 268 and name CA) (resid 268 and name CB)
      (resid 268 and name CG) (resid 268 and name CD1) 1 90.0 30.0 2
assign (resid 269 and name N) (resid 269 and name CA)
      (resid 269 and name CB) (resid 269 and name CG) 1 -60.0 60.0 2
20 assign (resid 269 and name CA) (resid 269 and name CB)
      (resid 269 and name CG) (resid 269 and name CD) 1 180.0 60.0 2
assign (resid 270 and name N) (resid 270 and name CA)
      (resid 270 and name CB) (resid 270 and name CG) 1 -60.0 60.0 2
25 assign (resid 270 and name CA) (resid 270 and name CB)
      (resid 270 and name CG) (resid 270 and name CD1) 1 180.0 60.0 2
assign (resid 272 and name N) (resid 272 and name CA)
      (resid 272 and name CB) (resid 272 and name OG1) 1 60.0 60.0 2
assign (resid 273 and name N) (resid 273 and name CA)
      (resid 273 and name CB) (resid 273 and name CG) 1 -60.0 60.0 2
30 assign (resid 273 and name CA) (resid 273 and name CB)
      (resid 273 and name CG) (resid 273 and name ND1) 1 90.0 30.0 2
assign (resid 275 and name N) (resid 275 and name CA)
      (resid 275 and name CB) (resid 275 and name CG) 1 -60.0 60.0 2
35 assign (resid 275 and name CA) (resid 275 and name CB)
      (resid 275 and name CG) (resid 275 and name OD1) 1 -60.0 60.0 2
assign (resid 276 and name N) (resid 276 and name CA)
      (resid 276 and name CB) (resid 276 and name CG1) 1 180.0 60.0 2
assign (resid 278 and name N) (resid 278 and name CA)
      (resid 278 and name CB) (resid 278 and name CG) 1 -60.0 60.0 2
40 assign (resid 278 and name CA) (resid 278 and name CB)
      (resid 278 and name CG) (resid 278 and name CD) 1 180.0 60.0 2
assign (resid 279 and name N) (resid 279 and name CA)
      (resid 279 and name CB) (resid 279 and name CG) 1 180.0 60.0 2
45 assign (resid 279 and name CA) (resid 279 and name CB)
      (resid 279 and name CG) (resid 279 and name CD) 1 180.0 60.0 2
assign (resid 280 and name N) (resid 280 and name CA)
      (resid 280 and name CB) (resid 280 and name CG) 1 -60.0 60.0 2
50 assign (resid 280 and name CA) (resid 280 and name CB)
      (resid 280 and name CG) (resid 280 and name CD1) 1 180.0 60.0 2
assign (resid 281 and name N) (resid 281 and name CA)
      (resid 281 and name CB) (resid 281 and name CG) 1 -60.0 60.0 2
assign (resid 281 and name CA) (resid 281 and name CB)
      (resid 281 and name CG) (resid 281 and name CD) 1 180.0 60.0 2
55 assign (resid 304 and name N) (resid 304 and name CA)
      (resid 304 and name CB) (resid 304 and name CG) 1 -60.0 60.0 2
assign (resid 304 and name CA) (resid 304 and name CB)
      (resid 304 and name CG) (resid 304 and name CD1) 1 90.0 30.0 2
assign (resid 305 and name N) (resid 305 and name CA)
      (resid 305 and name CB) (resid 305 and name CG) 1 180.0 60.0 2
60 assign (resid 305 and name CA) (resid 305 and name CB)
      (resid 305 and name CG) (resid 305 and name CD1) 1 180.0 60.0 2
assign (resid 306 and name N) (resid 306 and name CA)
      (resid 306 and name CB) (resid 306 and name CG) 1 -60.0 60.0 2
65 assign (resid 306 and name CA) (resid 306 and name CB)
      (resid 306 and name CG) (resid 306 and name OD1) 1 -60.0 60.0 2
assign (resid 307 and name N) (resid 307 and name CA)
      (resid 307 and name CB) (resid 307 and name CG) 1 -60.0 60.0 2
assign (resid 307 and name CA) (resid 307 and name CB)
      (resid 307 and name CG) (resid 307 and name SD) 1 180.0 60.0 2
70 assign (resid 308 and name N) (resid 308 and name CA)
      (resid 308 and name CB) (resid 308 and name CG1) 1 180.0 60.0 2
assign (resid 309 and name N) (resid 309 and name CA)
      (resid 309 and name CB) (resid 309 and name CG1) 1 180.0 60.0 2
75 assign (resid 310 and name N) (resid 310 and name CA)
      (resid 310 and name CB) (resid 310 and name CG) 1 -60.0 60.0 2
assign (resid 310 and name CA) (resid 310 and name CB)
      (resid 310 and name CG) (resid 310 and name OD1) 1 60.0 30.0 2
assign (resid 311 and name N) (resid 311 and name CA)
      (resid 311 and name CB) (resid 311 and name CG) 1 180.0 60.0 2
80 assign (resid 311 and name CA) (resid 311 and name CB)
      (resid 311 and name CG) (resid 311 and name CD) 1 60.0 30.0 2
assign (resid 312 and name N) (resid 312 and name CA)
      (resid 312 and name CB) (resid 312 and name OG1) 1 -60.0 60.0 2

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	assign	(resid 313 and name N)	(resid 313 and name CA)			
		(resid 313 and name CB)	(resid 313 and name CG)	1 -60.0	60.0	2
	assign	(resid 313 and name CA)	(resid 313 and name CB)			
5		(resid 313 and name CG)	(resid 313 and name CD1)	1 180.0	60.0	2
	assign	(resid 314 and name N)	(resid 314 and name CA)			
		(resid 314 and name CB)	(resid 314 and name CG)	1 180.0	60.0	2
	assign	(resid 314 and name CA)	(resid 314 and name CB)			
		(resid 314 and name CG)	(resid 314 and name CD)	1 180.0	60.0	2
10	assign	(resid 315 and name N)	(resid 315 and name CA)			
		(resid 315 and name CB)	(resid 315 and name CG)	1 -60.0	60.0	2
	assign	(resid 315 and name CA)	(resid 315 and name CB)			
		(resid 315 and name CG)	(resid 315 and name CD1)	1 180.0	60.0	2
	assign	(resid 316 and name N)	(resid 316 and name CA)			
		(resid 316 and name CB)	(resid 316 and name CG)	1 -60.0	60.0	2
15	assign	(resid 316 and name CA)	(resid 316 and name CB)			
		(resid 316 and name CG)	(resid 316 and name CD1)	1 90.0	30.0	2
	assign	(resid 323 and name N)	(resid 323 and name CA)			
		(resid 323 and name CB)	(resid 323 and name CG)	1 -60.0	60.0	2
20	assign	(resid 325 and name N)	(resid 325 and name CA)			
		(resid 325 and name CB)	(resid 325 and name CG1)	1 180.0	60.0	2
	assign	(resid 326 and name N)	(resid 326 and name CA)			
		(resid 326 and name CB)	(resid 326 and name SG)	1 -60.0	60.0	2
	assign	(resid 330 and name N)	(resid 330 and name CA)			
		(resid 330 and name CB)	(resid 330 and name CG1)	1 180.0	60.0	2
25	assign	(resid 337 and name N)	(resid 337 and name CA)			
		(resid 337 and name CB)	(resid 337 and name CG1)	1 -60.0	60.0	2
	assign	(resid 341 and name N)	(resid 341 and name CA)			
		(resid 341 and name CB)	(resid 341 and name CG)	1 -60.0	60.0	2
30	assign	(resid 342 and name N)	(resid 342 and name CA)			
		(resid 342 and name CB)	(resid 342 and name CG1)	1 180.0	60.0	2
	assign	(resid 343 and name N)	(resid 343 and name CA)			
		(resid 343 and name CB)	(resid 343 and name CG1)	1 180.0	60.0	2
	assign	(resid 345 and name N)	(resid 345 and name CA)			
		(resid 345 and name CB)	(resid 345 and name CG1)	1 -60.0	60.0	2
35	assign	(resid 347 and name N)	(resid 347 and name CA)			
		(resid 347 and name CB)	(resid 347 and name CG)	1 60.0	60.0	2
	assign	(resid 348 and name N)	(resid 348 and name CA)			
		(resid 348 and name CB)	(resid 348 and name CG)	1 180.0	60.0	2
40	assign	(resid 348 and name CA)	(resid 348 and name CB)			
		(resid 348 and name CG)	(resid 348 and name CD1)	1 90.0	30.0	2
	assign	(resid 350 and name N)	(resid 350 and name CA)			
		(resid 350 and name CB)	(resid 350 and name CG)	1 -60.0	60.0	2
	assign	(resid 350 and name CA)	(resid 350 and name CB)			
		(resid 350 and name CG)	(resid 350 and name CD1)	1 180.0	60.0	2
45	assign	(resid 352 and name N)	(resid 352 and name CA)			
		(resid 352 and name CB)	(resid 352 and name CG)	1 -60.0	60.0	2
	assign	(resid 352 and name CA)	(resid 352 and name CB)			
		(resid 352 and name CG)	(resid 352 and name CD)	1 180.0	60.0	2
	assign	(resid 353 and name N)	(resid 353 and name CA)			
50		(resid 353 and name CB)	(resid 353 and name CG)	1 180.0	60.0	2
	assign	(resid 355 and name N)	(resid 355 and name CA)			
		(resid 355 and name CB)	(resid 355 and name CG)	1 -60.0	60.0	2
	assign	(resid 355 and name CA)	(resid 355 and name CB)			
		(resid 355 and name CG)	(resid 355 and name CD)	1 180.0	60.0	2
55	assign	(resid 356 and name N)	(resid 356 and name CA)			
		(resid 356 and name CB)	(resid 356 and name CG)	1 -60.0	60.0	2
	assign	(resid 356 and name CA)	(resid 356 and name CB)			
		(resid 356 and name CG)	(resid 356 and name CD1)	1 90.0	30.0	2
	assign	(resid 363 and name N)	(resid 363 and name CA)			
60		(resid 363 and name CB)	(resid 363 and name CG)	1 180.0	60.0	2
	assign	(resid 363 and name CA)	(resid 363 and name CB)			
		(resid 363 and name CG)	(resid 363 and name CD1)	1 90.0	30.0	2
	assign	(resid 382 and name N)	(resid 382 and name CA)			
		(resid 382 and name CB)	(resid 382 and name CG1)	1 60.0	60.0	2
65	assign	(resid 384 and name N)	(resid 384 and name CA)			
		(resid 384 and name CB)	(resid 384 and name CG)	1 -60.0	60.0	2

```

    assign (resid 399 and name CB) (resid 399 and name CG) 1 -60.0 60.0 2
    assign (resid 399 and name CA) (resid 399 and name CB)
    assign (resid 399 and name CG) (resid 399 and name SD) 1 180.0 60.0 2
5  assign (resid 401 and name N) (resid 401 and name CA)
    assign (resid 401 and name CB) (resid 401 and name CG) 1 -60.0 60.0 2
    assign (resid 401 and name CA) (resid 401 and name CB)
    assign (resid 401 and name CG) (resid 401 and name SD) 1 180.0 60.0 2
    assign (resid 402 and name N) (resid 402 and name CA)
10  assign (resid 402 and name CB) (resid 402 and name CG) 1 180.0 60.0 2
    assign (resid 402 and name CA) (resid 402 and name CB)
    assign (resid 402 and name CG) (resid 402 and name CD) 1 180.0 60.0 2
    assign (resid 403 and name N) (resid 403 and name CA)
15  assign (resid 403 and name CB) (resid 403 and name CG) 1 -60.0 60.0 2
    assign (resid 403 and name CA) (resid 403 and name CB)
    assign (resid 403 and name CG) (resid 403 and name CD1) 1 180.0 60.0 2
    assign (resid 406 and name N) (resid 406 and name CA)
    assign (resid 406 and name CB) (resid 406 and name CG1) 1 -60.0 60.0 2
    assign (resid 407 and name N) (resid 407 and name CA)
20  assign (resid 407 and name CB) (resid 407 and name CG) 1 -60.0 60.0 2
    assign (resid 407 and name CA) (resid 407 and name CB)
    assign (resid 407 and name CG) (resid 407 and name CD) 1 180.0 60.0 2
    assign (resid 408 and name N) (resid 408 and name CA)
    assign (resid 408 and name CB) (resid 408 and name CG1) 1 180.0 60.0 2
    assign (resid 409 and name N) (resid 409 and name CA)
25  assign (resid 409 and name CB) (resid 409 and name CG) 1 -60.0 60.0 2
    assign (resid 409 and name CA) (resid 409 and name CB)
    assign (resid 409 and name CG) (resid 409 and name CD1) 1 180.0 60.0 2
    assign (resid 410 and name N) (resid 410 and name CA)
    assign (resid 410 and name CB) (resid 410 and name CG) 1 -60.0 60.0 2
30  assign (resid 410 and name CA) (resid 410 and name CB)
    assign (resid 410 and name CG) (resid 410 and name CD) 1 180.0 60.0 2
    assign (resid 415 and name N) (resid 415 and name CA)
    assign (resid 415 and name CB) (resid 415 and name CG) 1 -60.0 60.0 2
    assign (resid 415 and name CA) (resid 415 and name CB)
35  assign (resid 415 and name CG) (resid 415 and name CD) 1 180.0 60.0 2
    assign (resid 424 and name N) (resid 424 and name CA)
    assign (resid 424 and name CB) (resid 424 and name CG) 1 180.0 60.0 2
    assign (resid 424 and name CA) (resid 424 and name CB)
    assign (resid 424 and name CG) (resid 424 and name CD1) 1 180.0 60.0 2
40  assign (resid 439 and name N) (resid 439 and name CA)
    assign (resid 439 and name CB) (resid 439 and name CG1) 1 180.0 60.0 2

```

Legends

45

Figure 1: Structure-based alignment of human cytochrome P450 3A4 with bacterial P450 crystal structures, and rabbit P450 2C5.

Sequence numbering is indicated for each enzyme. This alignment is first based on the structural alignment of bacterial P450s and rabbit P450 2C5 derived from GOK
50 analysis. Human P450 3A4 sequence was then aligned with in-house tool (SmartConsAlign) that locates the CSBs on the target sequence, without introduction of any structural information for this complex. The alignment shown outside the CSBs is thus not relevant. The CSB sequences are indicated by bold uppercase characters and are highlighted in yellow. Amino acids strictly conserved
55 between CYP3A and 2C5, or between CYP3A and all the sequences of crystal structures, are highlighted in blue.

Figure 2: Ramachandran plot of a lowest energy model produced by DYANA-XPLOR calculations from the six-template structural alignment.

**Figure 3: view of one optimized CYP3A4 model. This figure can be replaced by
5 the whole set of coordinates file in the PDB format)**

Figure 4: final position of testosterone after soft-restrained restrained dynamics docking.

10 Figure 5: Energy profile of the soft-restrained restrained dynamics docking of testosterone into CYP3A4 model.

Example 1: Determination of the 3D-structure of P450 3A4.

15

Material

The coordinates of the six P450 crystal structures: P450cam (3cpp), P450terp (1cpt), P450BM-3 (2hpd), P450eryF (1oxa), P450 nor (1rom) and P450 2C5 (1dt6) were retrieved from the Brookhaven Protein data bank. The structural alignment
20 and the conserved regions determination were realized using the GOK software (Jean et al. 1997) running on an Octane Silicon-Graphics workstation. Structures were built using the DYANA (Güntert et al. 1997), and X-PLOR softwares (Brünger 1992). Docking studies were performed with SYBYL 6.6 (Tripos Inc.). The structures were analyzed using Procheck-NMR (Laskowski et al. 1993) and
25 visualized under SYBYL 6.6 (Tripos Inc.).

Common Structural Blocks (CBS) determination.

The first key point of this homology modeling study is the identification of the structural elements (hereafter designed as CSBs for Common Structural Blocks)
30 conserved among the family of cytochromes P450 of known 3D structures, and the localization of these elements in the target sequence. These two tasks are performed using the GOK software (Jean et al. 1997), and are well described in a forthcoming article (Minoletti et al., *Proteins, Structure, Function and Genetics*, 2002). In brief,

the basic idea of CSB identification by GOK is to use an internal coordinate representation – (α, τ) in our case (another representation of ϕ, ψ angles) – and to search for fragments in the six-template proteins having similar local trajectories in the internal coordinate space. GOK provides two adjustable parameters (the α -mesh
5 and the α -margin) that define the tolerance on the comparison of the trajectories. These parameters were adjusted recursively to values ranging from 15 to 30° (α -mesh) and 1 to 3 (α -margin in mesh units). The evaluation of the quality of the match was measured using two multiple-way rmsd calculated in the cartesian coordinates space: mp-rms (the mean of all pairwise rms deviations) and s-rms (the
10 mean of the deviations calculated with respect to a mean structure obtained from the average internal coordinates). For the different CSBs, mp-rms value ranged between 0.3 and 4.9 Å in average, and s-rms between 0.04 and 2.4 Å.

CYP3A4 sequence alignment and evaluation of the profile

15 The multiple sequence alignment derived from the CSB identification was then used to build a similarity profile. The profile is defined as a position-specific scoring table created from aligned gap-free segments such as CSBs (Jean et al. 1997). The alignment then consists in a search of the best match (as per the best score) between a CSB of sequences defined structurally (*i.e.* independently of the
20 nature of the aligned residues) and several other sequences that are well-aligned and exhibit a high sequence similarity. In the P450 3A subfamily, many proteins exhibit high sequence similarity. We extended our profile search program to take this information into account, *i.e.* to align the profile with a pre-defined multiple alignment of the cytochromes P450 3A subfamily members sequences (Gotoh 1992;
25 Nelson et al. 1996). The similarity score was calculated using BLOSUM62 matrix (Henikoff and Henikoff 1992; Loiseau 2002). The in-house tool SmartConsAlign (Atelier de Bio-informatique, Université Paris VI, <http://www.wabi.snv.jussieu.fr/~jompo>) allows to move the consensus matrix along the multiple sequence alignment of P450 3A family, and computes for each position
30 a score of similarity. The best alignment found of CYP3A4 on CSBs is shown in Figure 1 (Loiseau 2002).

Once the alignment is completed, the 3D model rebuilding process can incorporate the atom Cartesian coordinates of the template structures only for amino acids located in structurally conserved regions (*i.e.* the CSBs). The coordinates of any of the template structures can be used for the final template. In each CSB, amino acid positions have been renumbered according to the sequence of human P450 3A4. At a given position, when residues are identical between all the template structures and the target sequence, the 3D coordinates of the reference residues are purely assigned to the modeled (target) residue. When residues differ, only the coordinates of the backbone atoms are assigned ($C\alpha$), and sometimes $C\beta$ when they exist. Side chains are rebuilt from databanks giving the most probable rotamers for each amino acid (see below). In some cases, it was possible to superimpose the positions of carbon atoms of lateral chains up to ranks γ and δ , thus explicitly defining a unique rotamer.

For amino acids located outside the CSBs (structurally variable zones that include generally loops), the rebuilding is more complex, and can be done only after structurally conserved zones rebuilding. In the multiple structural alignment (fig. 1), the regions separating the CSBs bring no structural information at all. Short loops are rebuilt entirely, since solutions of acceptable geometry for atoms are in limited number, *i.e.* the lowest energy drives the selection of the good geometry. For longer segments, various structures are provided by the constrained minimization runs, and a manual selection is operated.

Constraints derivation and rebuilding

A strategy inspired of the techniques commonly used to built structures from NMR data (Patard et al. 1996) is applied. The main idea is to express all available information issued from the comparison of the templates in term of geometrical constraints (distances and angles). Each constraint will be defined as an interval (for a given pair of atoms, this is the average of the six atom-atom distances found in the template structures +/- the standard deviation), similarly to the strategy developed by Havel and Snow (Havel and Snow 1991). However, the number of constraints corresponding to all atom-atom distances, for example, would be prohibitive for a protein of the size of the P450 (around 1,000,000 inter-residual distances if we consider 250 conserved residues and four atoms by residues). Previous NMR

studies (Patard et al. 1996) have shown that local constraints are sufficient to allow a correct reconstruction of a structure. This reduces drastically the number of constraints needed, and increases the flexibility of the model. In addition, similarly to what is done in NMR, we can build a family of structures instead of a single model. This allows an easier analysis of the well or less well-predicted regions. This is also an advantage for the analysis of the side-chain positions, particularly in prevision of a substrate docking study. Finally, The loops are passively reconstructed with the rest of the structure. The only specific information we have introduced in variable regions was to guide all their residues to an allowed region of the Ramachandran diagram. Indeed, analysis of well-defined structures shows that nearly all residues, including those of the loops, should belong to an allowed region. The better the structure is, the lower the proportion of residue outside the allowed region. This criterion of quality has been applied to derive the model described herein.

Accordingly, we retained for model rebuilding all the distance and angle intervals corresponding to the following principles:

- all distances for which the lower bondary was less than 8 Å. This cutoff is totally sufficient to ensure, at least, the formation of the local structure elements. Such a cutoff is relatively high and thus costly in terms of size of constraints file, but proved necessary to ensure good results for the P450s. This may be due to the fact that P450 enzymes are mostly formed of α -helices, the average distance between two helices being larger than between two adjacent β -strands. In addition, the percentage of residues located outside CSBs is rather high in the structural alignment of P450s, and a better convergence can be obtained only at the expense of a high number of rebuilding distance constraints.
- all the distances involving at least one side-chain atom, to preserve the spatial arrangement between CSBs
- finally, all the distances involving atoms of the heme group, to fix as much as possible the neighborhood of the iron atom.

The total number of distance constraints was, in these conditions, equal to 58506 (Table 3).

Similarly, angular constraints were calculated in each building block. A CSB is indeed defined as a conserved trajectory in the ϕ, ψ coordinates space (or α, τ). Thus, dihedral angles ϕ and ψ of all residues located in CSBs can be defined as constraints, given by the average values of corresponding ϕ, ψ angles in the six
5 templates +/- the standard deviation. To these backbone dihedral angles, can be added the side chains torsion angles χ_1, χ_2 whenever possible, as determined by the rotamer selection. The total number of dihedral angle constraints was, in these conditions, equal to 761 (Table 4).

10 *Rotamer selection*

In proteins, the preferential orientation of the side chain ($60^\circ, -60^\circ, 180^\circ$) depends on the local conformation of the residue, and thus on the nature of the secondary structure in which the residue is involved. According to the rotamer library built by Karplus and coll. (Dunbrack and Karplus 1993), to a given (ϕ, ψ) couple in the
15 Ramachandran diagram can be associated a specific rotamer. These tables have been used to determine the most probable rotamer for each residue located in CSB, except when there are conserved atoms in the side chain that assign unambiguously a rotamer (χ_1, χ_2) . The selected (χ_1, χ_2) couples are reported in the dihedral constraints of Table 4.

20

Structure calculation and optimization

We used a procedure similar to structure calculation starting from NMR constraints. A first set of structures was calculated using the DYANA software (Güntert et al. 1997) and the two constraints Tables 4 and 3. It must be pointed out that these
25 Tables represent the scaffold for rebuilding any of the CYP3A that can be aligned (Figure 1). Families of structures are generated. The energy of each structure is minimized with the procedure vtfmin in DYANA.

Due to the size and the amount of loops in the molecule, some structures presented topological defects and were discarded. The others were further optimized by using
30 the X-PLOR software. A set of constraints was added at this stage in order to guide the loop residues to the nearest allowed region in the Ramachandran diagram. The

topology and parameter files of CHARMM22 were used. The electrostatic term was turned off.

The DYANA software is unable to deal with disconnected objects. A new residue type was, thus, added to the standard amino acid library to take into account the presence of the heme. This residue was obtained by combining the heme to a
5 cysteine and was inserted at position 441 in the sequence of the protein (Figure 1).

Description of the CYP3A4 Model

10 We rebuilt a model of the protein depleted of its first 50 residues (N-terminal domain). This segment is highly hydrophobic, and supposed to form the anchor of the protein in the membrane. There is no structural information about this putative transmembrane domain, and this segment was thus not incorporated into the modeling process, and in the final model. Such a “free” segment (with no
15 constraints) would perturb the convergence of computation or the stability of the whole rebuilt structure.

The quality of the various structures optimized under XPLOR was checked for the stereochemical quality (backbone and side chain conformation) by PROCHECK
20 (Laskowski et al. 1993). The Ramachandran plot shows that our six-template approach generated converging models, possessing the same fold. The lowest energy models had 73% of their non-glycine and non-proline residues with ϕ , ψ conformation in the most favoured regions of the Ramachandran plot (core region), 20% in additional allowed regions, and 5% in the generously allowed regions. Only
25 2.3% (9 residues) had their ϕ , ψ conformation in disallowed regions (Figure 2). The total number of residues in the model is 452; which 399 are non-glycine and non-proline residues, and number of residues in the native sequence is 502.

When compared to the CYP2C5 crystal structure, it can be noticed that the
30 CYP3A4 model exhibits a good 3D similarity in the global fold than expected, since this structure counts only for one in the six-template approach. This proves that in this approach, there is no “averaging” effect, *i.e.* the mammalian structure had a decisive influence over the five bacterial (and fungus) templates. Our final fold of

CYP3A4 is very consistent with a mammalian one, despite the fact that it has been rebuilt by using the structural information contained in non-mammalian cytochromes P450.

- 5 The active site is delimited by the six substrate recognition sites (SRS) that have been first identified and described by Gotoh (Gotoh 1992) from the unique structure available in the early 1990s (P450_{cam}), and that are today commonly accepted for depicting substrate recognition by various cytochromes P450 (especially from the family 2, but extended to other P450 families). These sites are associated with the
- 10 active site and are located in the less conserved regions of the CYPs, thus possibly accounting for the various substrate specificity among P450s. When comparing our various optimized structures, it is found that SRS1 (100-125, includes helix B), SRS 2 (205-218, includes C-terminus of helix F), and SRS3 (237-249, includes N-terminus part of helix G) are located in less-defined regions, with significant
- 15 variability in spatial position (flexibility). These regions correspond also to parts of the sequence that are less well-aligned. At the opposite, the SRS4 (295-320, central part of helix D), SRS5 (363-380, C-term of helix K and β -sheet β 1-4) and SRS6 (470-490, β -sheets β 4-1 and β 4-2) are well-defined fragments of the structures. SRS4 and SRS5 segments in particular are correlated to regions in the sequence that
- 20 are unequivocally aligned.

The only model structure of CYP3A4 that has been described in the literature and that we can handle for structural comparison, is that of Szklarz and Halpert, derived

25 from a multiple-template approach (four-bacterial template) (Szklarz and Halpert 1997). Roughly, the same secondary structures are identified, but we found divergences in SRS location between their model and those derived from the present approach. SRS4 and SRS5 match well, but SRS2 is shifted (divergence in the position of helix F along the sequence), while SRS1 (helix B'), SRS3 (helix G)

30 and SRS6 (sheet β 4) are more notably displaced. The loops connecting the secondary structures of these SRS significantly disagree. These differences are likely to issue from a wrong alignment with the crystal P450 structures in the model of Szklarz and Halpert..

Example 2: Docking Strategy

5 Our aim was to obtain the different positions of the known substrates of CYP3A4 in the active site, consistent with the oxidation sites. Considering the fact that the heme-binding site is deeply buried in the protein structure, and thus the selection and the pathway of the substrates within the enzyme structure are strongly dependent on the various possibilities of structure opening, we implemented a
10 special approach more appropriate to flexible structures, hereafter referred as “restrained dynamics docking” or “soft-restrained restrained dynamics docking”. This technique employs constrained dynamics simulations, where the only constraints are heme-substrate distances. The successive steps are:

15 *Conversion of the PDB XPLOR file in PDB for SYBYL file*

The optimized structures with XPLOR (PDB format) are visualized with the SYBYL 6.6 software (Tripos Inc.), which implies a conversion of the file (atoms types correction) so as to make it compatible and exploitable in the constrained dynamics which will be performed with SYBYL.

20

Stabilisation du modèle de P450 3A généré sous XPLOR

Then, we do agregate N°1 (in the meaning of SYBYL) with all the NC_αCO atoms of the peptide backbone of the protein. The structure is relaxed with a dynamic of 10ns at 100K followed by a une minimization of 100 pas. Agregate N°1 is then
25 deleted.

We do agregate N°2 constituted of the protein C_α only. The protein relaxation is reiterated with a dynamic of 10 ns at 100K and une minimization of 100 pas. Agregate N°2 is then deleted.

30

The all protein is then relaxed with a first dynamic of 1ns at 100K, followed by a dynamic of 1ns at 200K and a dynamic of 10ns at 300K. We terminate with a minimization of 100 pas.

Restrained dynamics docking of the substrate (example: testosterone)

We do aggregate N°3 constituted of all atoms outside a sphere of 20Å around the C_α of residues constituting the heart of the B' loop. We also add hematic iron to this
5 aggregate.

The substrate is placed inside the protein, at around 30Å from the hematic iron and next to SRS1 and SRS5 sites. The substrate is placed so that the constraints between the hematic iron and the substrate backbone go between SRS1, SRS5 and SRS3. Thus, when testosterone is docking, we establish 4 distance constraints (limit below
10 3Å, above 10Å) between hematic iron and C3, C8, C10 and C13 carbones with a constrain of 2 kcal/Å on the entire structure so as to avoid to favour the approach of one part of the substrate more than the other.

We begin to perform a dynamic without constraints of the entire system at 20 K
15 during 2ns to stabilize the system, then we perform a dynamic under constraints at 20 K during 5ns. We observe that the substrate worms between SRS1, SRS3 et SRS5 to reach a position at the vicinity of hematic iron. We terminate with a dynamic without constraints at 300 K to relax the system and we realize a minimization of 1000 pas.

20

Results

We found that the testosterone molecule is positioned at the vicinity of hematic iron in such way that the C6 of testosterone be at 4.9Å of the iron, which is compatible with the hydroxylation of this compound to give 6β-hydroxy-testosterone (Figure
25 4).

Minimizations and dynamics with the SYBYL software are performed with the Tripos force field following the parameters: dielectric constant equal to 1 and distance-dependent, minimization method of POWELL, a minimum gradient of 0.05kcal.mol⁻¹.Å⁻¹, electrostatics charges calculated according to the Gasteiger-
30 Hückel method, and a NB cutoff of 8.0Å (non-bond energies). The energetic diagram of dynamic docking of testosterone is shown in Figure 5.

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References

- Brünger, A.T. 1992. X-PLOR Version 3.1. A system for X-ray crystallography and
5 NMR.
- Chothia, C., and Lesk, A.M. 1986. The relation between the divergence of sequence
and structure in proteins. *Embo J* 5: 823-826.
- Cupp-Vickery, J.R., and Poulos, T.L. 1995. Structure of cytochrome P450eryF
involved in erythromycin biosynthesis. *Nature Struct. Biology* 2: 144-153.
- 10 Dunbrack, R.L.J., and Karplus, M. 1993. Backbone-dependent rotamer library for
proteins- Application to side chain prediction. *J. Mol. Biol.* 230: 543-574.
- Ferenczy, G., and Morris, G. 1989. The active site of cytochrome P450 nifedipine
oxidation model building study. *J. Mol. Graph.* 7: 206-211.
- Gotoh, O. 1992. Substrate Recognition Sites in Cytochrome-P450 Family-2 (CYP2)
15 Proteins Inferred from Comparative Analyses of Amino Acid and Coding
Nucleotide Sequences. *Journal of Biological Chemistry* 267: 83-90.
- Güntert, P., Mumenthaler, C., and Wüthrich, K. 1997. Torsion angle dynamics for
NMR structure calculation with the new program DYANA. *J. Mol. Biol.*
273: 283-298.
- 20 Hasemann, C.A., Ravichandran, K.G., Peterson, J.A., and Deisenhofer, J. 1994.
Crystal Structure and Refinement of Cytochrome P450(Terp) at 2.3 Å
Resolution. *J. Mol. Biol.* 236: 1169-1185.
- Havel, T.F., and Snow, M.E. 1991. A new method for building protein
conformations from sequence alignments with homologues of known
25 structure. *J Mol Biol* 217: 1-7.
- Henikoff, S., and Henikoff, J.G. 1992. Amino acid substitution matrices from
protein blocks. *Proc Natl Acad Sci USA* 89: 10915-10919.
- Hilbert, M., Bohm, G., and Jaenicke, R. 1993. Structural relationships of
homologous proteins as a fundamental principle in homology modeling.
30 *Proteins* 17: 138-151.
- Jean, P., Pothier, J., Dansette, P.M., Mansuy, D., and Viari, A. 1997. Automated
multiple analysis of protein structures: application to homology modeling of
cytochromes P450. *Proteins* 28: 388-404.

- Laskowski, R.A., MacArthur, M., Moss, D.S., and Thornton, J. 1993. PROCHECK: a program to check the stereochemical quality of protein structures. *J. Appl. Crystallog.* **26**: 283-291.
- Lewis, D.F.V. 2001. *Guide to cytochrome P450 structure and function*. Taylor & Francis, New York, pp. cm.
- Lewis, D.F.V., Eddershaw, P.J., Goldfarb, P.S., and Tarbit, M.H. 1996. Molecular modelling of CYP3A4 from an alignment with CYP102: Identification of key interactions between putative active site residues and CYP3A-specific chemicals. *Xenobiotica* **26**: 1067-1086.
- 10 Loiseau, N. 2002. Conception d'analogues structuraux d'un cyclopeptide modèle: étude du mode de reconnaissance moléculaire par trois systèmes enzymatiques membranaires. Université Paris XI, Orsay.
- Nelson, D.R. 1999. Cytochrome P450 and the individuality of species. *Arch Biochem Biophys* **369**: 1-10.
- 15 Nelson, D.R., Koymans, L., Kamataki, T., Stegeman, J.J., Feyereisen, R., Waxman, D.J., Waterman, M.R., Gotoh, O., Coon, M.J., Estabrook, R.W., et al. 1996. P450 superfamily: Update on new sequences, gene mapping, accession numbers and nomenclature. *Pharmacogenetics* **6**: 1-42.
- Park, S.Y., Shimizu, H., Adachi, S., Nakagawa, A., Tanaka, I., Nakahara, K., Shoun, H., Obayashi, E., Nakamura, H., Iizuka, T., et al. 1997. Crystal structure of nitric oxide reductase from denitrifying fungus *Fusarium oxysporum*. *Nature Struct. Biology* **4**: 827-832.
- 20 Patard, L., Stoven, V., Gharib, B., Bontems, F., Lallemand, J.Y., and De Reggi, M. 1996. What function for human lithostathine? Structural investigations by three-dimensional structure modeling and high-resolution NMR spectroscopy. *Protein Eng* **9**: 949-957.
- 25 Podust, L.M., Poulos, T.L., and Waterman, M.R. 2001. Crystal structure of cytochrome P450 14alpha -sterol demethylase (CYP51) from *Mycobacterium tuberculosis* in complex with azole inhibitors. *Proc Natl Acad Sci USA* **98**: 3068-3073.
- 30 Poulos, T.L., Finzel, B.C., Gunsalus, I.C., Wagner, G.C., and Kraut, J. 1985. The 2.6 Å crystal structure of *Pseudomonas putida* cytochrome P450cam. *J. Biol. Chem* **260**: 16122-16130.

- Raag, R., and Poulos, T.L. 1989. Crystal structure of the carbon monoxide-substrate-cytochrome P-450cam ternary complex. *Biochemistry* **28**: 7586-7592.
- Ravichandran, K.G., Boddupalli, S.S., Hasemann, C.A., Peterson, J.A., and Deisenhofer, J. 1993. Crystal Structure of Hemoprotein Domain of P450BM-3, a Prototype for Microsomal P450's. *Science* **261**: 731-736.
- 5 Sanchez, R., Pieper, U., Melo, F., Eswar, N., Marti-Renom, M.A., Madhusudhan, M.S., Mirkovic, N., and Sali, A. 2000. Protein structure modeling for structural genomics. *Nat Struct Biol* **7 Suppl**: 986-990.
- Szklarz, G.D., and Halpert, J.R. 1997. Molecular modeling of cytochrome P450 3A4. *J Comput Aid Molec Design* **11**: 265-272.
- 10 Williams, P.A., Cosme, J., Sridhar, V., Johnson, E.F., and McRee, D.E. 2000. Mammalian microsomal cytochrome P450 monooxygenase: structural adaptations for membrane binding and functional diversity. *Molecular Cell* **5**: 121-131.
- 15 Yano, J.K., Koo, L.S., Schuller, D.J., Li, H., Ortiz de Montellano, P.R., and Poulos, T.L. 2000. Crystal structure of a thermophilic cytochrome P450 from the archaeon *Sulfolobus solfataricus*. *J Biol Chem* **275**: 31086-31092.

Claims

- 5 1. A method for designing a 3-dimentional (3-D) model of a protein, the 3-
dimensional representation of at least three family members has already been
experimentally obtained, [said 3-dimentional representation presenting
similarities], comprising the steps of:
 - a. identification of common structural blocks (CSB) among said members of said
 - 10 family,
 - b. alignment of the amino-acids primary sequence of said family members
according to said structural similarities, represented by said CSBs, in order to
obtained a first alignment,
 - c. alignment of said protein as compared on said first alignment, in order to obtain a
 - 15 second alignment, wherein:
 - i. alignment of said protein is performed in order to maximize the
amino-acids alignment between said protein and said first alignment,
when one or more consensus amino-acid exists in said aligned
structural blocs in said first alignment, and in the amino-acid
 - 20 sequence of said protein, said consensus amino-acids are anchors
of said second alignment,
 - ii. no insertion or deletion of amino-acids can be performed in the
aligned CSBs, wherein insertion or deletions are possible in non-aligned
structural blocks, if better to align the primary amino-acids sequences,
 - 25 d. definition of the atomic 3-D structure of structural blocs of said protein,
according to the 3-D structure of the blocks of said family members,
 - e. definition of the local constraints (distance and angles) for the atoms that are
not structurally determined after step d. (that are not in the conserved structural
blocks),
 - 30 f. selection of rotamers,
 - g. determination of a family of whole 3-D model structures of said protein,
taking into account said atomic 3-D structure of structural blocs obtained in step d.,
said local constraints defined in step e., and said rotamers defined in step f.,

- h. optimization of said family of 3-D models obtained in step g., by
- i. discarding sequences that present topological defects, and
 - ii. recalculating 3-D structures by taking electrostatic forces into account, and performing the method again from step c. downward, with modifications in the alignment between the primary sequence of said protein and said first alignment, when the obtained model structures do not take into account known mutations having biological effects.
2. The method of claim 1, wherein said 3-dimensional representation of family members has been obtained by crystallography or NMR.
3. The method of claim 1, wherein said alignment of said common structural blocks in step b. is performed by use of the GOK software as described in Jean et al., 1997.
4. The method of claim 1, wherein said alignment of said common structural blocks in step c. is performed by use of the GOK software as described in Jean et al., 1997.
5. The method of claim 1, wherein step d. is performed according to the following rules:
- i. at a given position, when residues are identical between all the template structures and the target sequence, the 3D coordinates of the reference residues are purely assigned to the target residue,
 - ii. When residues differ, only the coordinates of the backbone atoms are assigned ($C\alpha$), and sometimes $C\beta$ when they exist.
6. The method of claim 1, wherein said definition of local constraints in step e. is performed by analysis of the allowed regions in Ramachandran diagram.
7. The method of claim 1, wherein distances and angles are selected in step e. by the following rules:
- i. all distances for which the lower boundary was less than 8 Å.
 - ii. all the distances involving at least one side-chain atom, to preserve the spatial arrangement between CSBs
 - iii. all the distances involving atoms of any active group such as an heme group, to fix as much as possible the neighborhood of said active group, such as an iron atom.

8. The method of claim 1, wherein angular constraints are selected in step e. by the following rule:
 - i. dihedral angles ϕ and ψ of all residues located in CSBs are defined as constraints, given by the average values of corresponding ϕ , ψ angles in said family members +/- the standard deviation
9. The method of claim 1, wherein said rotamers in step f. are selected from the couples according to the tables of Dunbrack and Karplus, where the choice of rotamers of a given amino acid is guided by the most favored zones in Ramachandran χ_1 , χ_2 maps.
10. The method of claim 1, wherein said step g. is performed with the DYANA software, as described in Güntert et al, 1997.
11. The method of claim 1, wherein said optimization in step h. comprises the use of the X-Plor software, as described in A. T. Brünger, X-PLOR, version 3.1. A system for X-ray crystallography and NMR, Yale University Press, New Haven, CT (1992) and A. T. Brünger, Molecular replacement with X-PLOR: PC-refinement and free R value. In: Proceedings of the Daresbury Study Weekend on Molecular Replacement, Daresbury, United Kingdom (1992), 49-61.
12. The method of claim 1, wherein said protein is a cytochrome P450.
13. The method of claim 12, wherein said protein is cytochrome P450 3A4 (SEQ ID N° 1)
14. The method of claim 12, wherein said family members that are used for performing said first alignment are chosen from Nor, (SEQ ID N° 2), Ery F (SEQ ID N° 3), terp (SEQ ID N° 4), Cam (SEQ ID N° 5), BM3 (SEQ ID N° 6) and 2C5 (SEQ ID N° 7).
15. A model 3-D structure of a protein, obtained by the method according to claim 1.
16. The model of claim 15, wherein said protein is cytochrome P450 3A4.
17. The model of claim 16, wherein the residues C97; R104; F101; F107; F247; F303 and C376 are responsible for the recognition of the substrate at the entry site and into the active site.
18. The model of claim 16, having the three dimensional atomic coordinates of Table 1, for C- α , and the (ϕ , ψ) couples of Table 2.

19. A method for designing a protein, biological functions of which are altered, comprising:
 - a) obtaining a 3-D model of said protein by the method of claim 1,
 - b) analyzing said model of step a., and determining the amino-acids that are putatively involved in the biological functions of said protein,
 - c) changing said amino-acids by mutating the corresponding nucleotides on the nucleic acid sequence coding for said protein, in order to obtain a mutated protein having altered properties.
20. A computer-assisted method for performing restrained dynamics docking of a substrate on an enzyme, a 3-D structure of which is available, comprising the steps of
 - j. determining a force field, and independently simulating the presence of said enzyme in said force field,
 - k. minimizing the potential energy (Ep) linked to said force field of said 3-D structure, wherein the spatial position some atoms of said enzyme is fixed, and wherein the other atoms are mobile, by allowing mobility of the mobile atoms, by
 - i. simulating an increase in temperature (in order to give kinetic energy),
 - ii. and minimizing the potential energy by re-specifying the temperature as 0 Kelvin (K)
 - l. optionally repeating step b in order to obtain other Ep minima, wherein said Ep minima are such that the structure of the protein remains folded,
 - m. minimizing Ep in said force field of said 3-D structure, wherein all the atoms of the protein are mobile, by
 - i. simulating an increase in temperature (in order to give kinetic energy), and
 - ii. minimizing the potential energy by re-specifying the temperature as 0 Kelvin (K)
 - n. simulating, at 0 K the presence of said substrate next to said enzyme,
 - o. optionally generating a dynamic on said substrate and enzyme (simulating an increase in temperature, in order to allow mobility of the atoms)

- p. generating some constraints to said substrate, in order to impose that it has interaction with said enzyme,
- q. generating a dynamic on said substrate and enzyme, with said constraints imposed in step p.,
- 5 r. optionally, generating a dynamic on said substrate and enzyme without said constraints of step p.
- 21. The method of claim 20, wherein said fixed atoms in step k. are the backbone atoms N-C α -CO in the first minimization step and only C α in subsequent minimization steps.
- 10 22. The method of claim 20, wherein said kinetic energy is simulated by temperature increase to about 100 K for about 5-20 ns.
- 23. The method of claim 20, wherein said force field in step j. comprises forces linked to
 - a. the distance between atoms,
 - 15 b. the angles of valence,
 - c. the diedric angles,
 - d. the deformation with regard to plan,
 - e. the electrostatic field,
 - f. the Van der Waals forces,
 - 20 g. hydrogen bonds.
- 24. The method of claim 20, wherein said constraints in step p. are attraction constraints to force said substrate in the active site, and wherein said constraints are not prejudiced to the exact spatial conformation of the substrate in the active site.
- 25 25. The method of claim 24, wherein said constraints are final distance constraints between some atoms of said substrate and some atoms of amino-acids present in said active site.
- 26. The method of claim 20, wherein step o. is performed with a simulated temperature of between about 15 and 50 K.
- 30 27. The method of claim 20, wherein step q. is performed with a simulated temperature of between about 15 and 50 K.
- 28. The method of claim 20, wherein step r. is performed with a simulated temperature of between about 200 and 350 K.

29. The method of claim 20, wherein said enzyme is a cytochrome P450.
30. The method of claim 21, wherein said cytochrome is cytochrome P450 3A4, and said structure is the structure obtained by the method of claim 13, in particular the model structure of claim 18.
- 5 31. The method of claim 29, wherein said substrate is a small organic compound which size can range for example from MW 288 (testosterone) to MW 1203 (cyclosporine A).
32. The method of claim 31, wherein said substrate is testosterone.
- 10 33. A computer-assisted method for performing restrained dynamics docking of at least two substrates on an enzyme, a 3-D structure of which is available, comprising the steps consisting of performing the steps depicted in claim 20 with a first substrate and repeating said steps with a second substrate when the first substrate reaches an unconstrained molecular dynamic.
- 15 34. The method of claim 33, wherein the first and second substrates are the same molecule.
35. The method of claim 33, wherein the first and second substrates are different molecules.
36. The method of claim 34, wherein the first and second substrates display an
20 allosteric effect.
37. The method of claim 34, wherein the first and second substrates display a synergistic effect.
38. The method of claims 34 and 35, wherein at least one of the substrates is an inhibitor or display an inhibitor-base mechanism.
- 25 39. The method of claims 34 and 35, wherein at least one of the substrates is an agonist.
40. The method of claim 33 comprising successively repeating the steps of claim 20 with a 3rd, 4th or 5th substrate, some of them being the same or different molecules.
- 30 41. The method of claim 33, wherein said fixed atoms in step k. are the backbone atoms N-C α -CO in the first minimization step and only C α in subsequent minimization steps.

42. The method of claim 33, wherein said kinetic energy is simulated by temperature increase to about 100 K for about 5-20 ns.
43. The method of claim 33, wherein said force field in step j. comprises forces linked to
 - 5 a. the distance between atoms,
 - b. the angles of valence
 - c. the diedric angles,
 - d. the deformation with regard to plan,
 - e. the electrostatic field,
 - 10 f. the Van der Waals forces
 - g. hydrogen bonds
44. The method of claim 33, wherein said constraints in step p. are attraction constraints to force said substrate in the active site, and wherein said constraints are not prejudiced to the exact spatial conformation of the substrate in the active site.
- 15 45. The method of claim 44, wherein said constraints are final distance constraints between some atoms of said substrate and some atoms of amino-acids present in said active site.
46. The method of claim 33, wherein step o. is performed with a simulated temperature of between about 15 and 50 K.
- 20 47. The method of claim 33, wherein step q. is performed with a simulated temperature of between about 15 and 50 K.
48. The method of claim 33, wherein step r. is performed with a simulated temperature of between about 200 and 350 K.
- 25 49. The method of claim 33, wherein said enzyme is a cytochrome P450.
50. The method of claim 49, wherein said cytochrome is cytochrome P450 3A4, and said structure is the structure obtained by the method of claim 13, in particular the model structure of claim 18.
51. The method of claim 33, wherein said first and second substrates are small organic compounds which size can range from MW 288 (testosterone) to MW 1203 (cyclosporine A).
- 30 52. The method of claim 51, wherein said substrate is testosterone.

53. The use of the method according to claim 20 or 33 for screening, designing or identifying natural, unnatural substrates or substrate analogs, as well as inhibitors, activators or modulators of said enzyme.
54. The use of the method according to claim 33 or 40 for determining the effect
5 of a first substrate on a second substrate.
55. The use according to claim 54 applied to pharmaceutical products.
56. The use of the method according to claim 33 or 40 for determining the effect of a first testosterone molecule on a testosterone molecule.
57. The use of the method according to claim 33 or 40 for determining the effect
10 of a testosterone molecule on alpha-naphtoflavone.
58. The use of the method according to claim 20 to 40 for determining the oxidative modification of the substrate according to the proximity to the heme of a part of the substrate.
15
59. The oxidized or reduced molecule derived from a given substrate modified after positioning at the right distance to the heme is called metabolite
60. The use of the method according to claim 20 to 32, or 33 to 40, for
20 performing dynamic docking of the said metabolite, either in the absence or in the presence of the second substrate in the calculation.
61. The use of the method dynamic docking to compare the energy of the bound metabolite relatively to the energy of its parent substrate bound, in order to
25 determine if the exit of the given metabolite from the enzyme is favored or not.

SEQUENCE LISTING

SEQ ID No 1

- 5 CYP 3A4 human
Numbering starts at Ala 1 (first residue Met is not included,
consistently with SwissProt CP34_HUMAN P08684)
- 1 alipdlamet wlllavslvl lylygthshg lfkklgipgp tplpflgnil
10 syhkgfcmfd
- 61 mechkkygkv wgydgqqpv laitdpdmik tvlvkecysv ftnrrpfgpv
gfmksaisia
- 15 121 edeewkrlrs llsptftsgk lkemvpiaaq ygdvlvrnlr reaetgkpv
lkdvfgaysm
- 181 dvitstsfgv nidslnnpqd pfventkkll rfdfldpffl sitvfpflip
ilevlnicvf
- 20 241 prevtnflrk svkrmkersl edtqkhrvdf lqlmidsqns keteshkals
dlelvaqsii
- 301 fifagyetts svlsfimyel athpdvqqkl qeeidavlpn kapptydtvl
25 qmeyldmvvn
- 361 etlrlfpam rlercvckdv eingmfipkg wvwmipsyal hrdpkywtep
ekflperfsk
- 30 421 knkdnidpyi ytpfgsgprn cigmrfalnn mklalirvlq nfsfkpck
qiplklslgg
- 481 llqpekpvvl kvesrdgtvs ga

Title. A METHOD FOR PERFORMING
RESTRAINED DYNAMICS DOCKING OF
ONE OR MULTIPLE SUBSTRATES ON
MULTI-SPECIFIC ENZYMES
Inventor(s): Francois Andre et al.
Appl. No.: Unassigned

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1	Nor	-----	-----	-----	-----	masgap	sfpfsrasgp	(16)		
2	Ery F	-----	-----	-----	-----	matvp	dLe-sdsfhv	(14)		
3	Terp	-----	-----	-----	mda	ratipehiar	tvilpqgyad	(23)		
4	Cam	-----	-----	-----	tteti	snanlaplpp	hvpelhvdf	dmynpsnlisa	(36)	
5	BM3	-----	-----	-----	t	ikempqpktf	gelknplln	(21)		
6	2C5	-----	-----	-----	makkt	sskgklppgp	tpfflignil	(43)		
7	CPC5_RABIT	-----	mdpv	vvlvlgclcl	lllsiwkqns	grgkl-pggp	tpfflignil			
8	CPC3_RABIT	-----	mdll	iilgiclscl	vllslwkkth	gkgkl-pggp	tpfflignil			
9	CPC1_RABIT	-----	-----	lsc1	llslwkqsy	gggkl-pggp	tpfflignil			
10	CP31_RAT	dllsaltlet	wlllavvlvl	lygfgtrthg	lfkkggipgp	kplpffgtvl	tpfflignil			
11	CP33_HUMAN	alipdlamet	wlllavslvl	lylygthshg	lfkklgipgp	tpfflignil		(50)		
12	CP34_HUMAN	alipdlamet	wlllavslvl	lylygthshg	lfkklgipgp	tpfflignil				
1		e-----	ppAEFA	KLRAt-----	n	PVSQVKLEdg	slawlvtkhk	DVCFvatse-	(58)	
2		d-----	WYST	YAEIret-----	a	PVTEVRFD	g	QAWLYTGID	EAKAalsdl-	(55)
3		d-ev-----	TYPA	FKWlrde-----	q	PLAMAHTEgy	dpmwIATKHA	DVMQlgkqpg	(68)	
4		g-----	VOEA	WAVIqesnvp	DLVWTRCNg-	GHWTATRGQ	LIREA	vedyr	(79)	
5		t-d-k-----	PVOA	LMKadcl-g	EIKFEAE-g	rvTRYLSSOR	LIKEAc-des	(67)		
6		qidakdISKS	LTKFsegvg	FVETVYLgmk	PTVVLHGYE	AVKEA	vdldg	(91)		
7		qidakdISKS	LTKFsegvg	FVETVYLgmk	PTVVLHGYE	AVKEA	vdldg			
8		qletkdINKS	LSMLakevg	SIFTLYFgmk	PAVVLGYE	GVIEA	ldrg			
9		qigiqdISKS	FTKLsevg	FVETVYLgmk	PTVVLHGYD	AVKEA	vdldg			
10		nyy-mgLWKF	DVEchkkvg	KIWGLFDgqm	ELFAITDTE	MIKNV	vkec			
11		syh-kgFCMF	DMEchkkvg	KVWGFYDgqq	EVLAITDTE	MIKLV	vkec			
12		syh-kgFCMF	DMEchkkvg	KVWGFYDgqq	EVLAITDTE	MIKLV	vkec	(97)		
		CSB 1*		CSB 1**		CSB 1				
1		klskvr-----	trqgfpel	-----	SASGKa	a-----	ka	-kptFVDMDE	(91)	
2		rlssdpkky	pgvevefpay	lgfPEDVRN	-----	y	fatNMGTSDE	(95)		
3		lfsnae-----	gse	ilyDONNEaf	mrsisggcph	vidSLTSMDE	(107)			
4		hfsse-----	cpfi	-----	PREAGE	-----	a	ydfIFTSMDE	(105)	
5		rfdknl-----	SOALKEv	r-----	df	agcGLFTSWT	(91)			
6		eefagr-----	gSVPILEk	vs-----	kgLGIAFSNA	(117)				
7		eefagt-----	gSVPILEk	vs-----	kgLGIAFSNA					
8		eefsgv-----	gIFPVFDr	vt-----	kgLGIVFSSG					
9		eefsgv-----	ivFELTAK	in-----	kgYGIVFSNG					
10		fsvftn-----	RRDFGPv	gi-----	mgkAVSVAKD					
11		ysvftn-----	REPFGPv	gf-----	mksAISIAED					
12		ysvftn-----	REPFGPv	gf-----	mksAISIAED	(122)				
		CSB 2A*		CSB 2A**						
1		PEHMQRS	MVEPTtpea	vk-----	nLOPYI	ORTVDDILEQ	MKQKgcang	(137)		
2		PTHTRLRK	LVSQESTvrr	-----	VEAMR	PRVEQITAEI	LDEvgds-gv	(137)		
3		PTHTAARG	LTLNWfpas	ir-----	KLEENI	RRIAQASVQR	LIDE-d-ge	(150)		
4		PEQORFRA	LANQVvgmpv	vd-----	KLENRI	QELACSLIES	LIRPO-----	gq	(147)	
5		heKNWKAHN	LLPSTsqqa	mk-----	gTHAMM	VDIAVOLVOK	WERIn-adeh	(138)		
6		KTWKEMRR	FSIMTLrnfg	mgkrsIEDRI	QEEARCLVEE	LRKTN--as	(163)			
7		KTWKEMRR	FSIMTLrnfg	mgkrsIEDRI	QEEARCLVEE	LRKTN--as				
8		EKWKETRR	FSLTVLrnlg	mgkrtIEERI	QEEALCLIOA	LRKTN--as				
9		KRWKETRR	FSIMTLrdfg	mgkrsIEDRV	QEEARCLVEE	LRKTN--gs				
10		EEWKRYRA	LLSPTftsg	rlk-eMFPII	EQYGDILVKY	LKQEAetgk				
11		EEWKRLRS	LLSPTftsg	klk-eMVPPII	AOYGDVLVRN	LRREretgk				
12		EEWKRLRS	LLSPTftsg	klk-eMVPPII	AOYGDVLVRN	LRREretgk	(168)			
		CSB 2A		CSB 2B						
1		VDLVKEFALE	NPSYIITLL	GVE-----	ENDLEYL	TOONAIRtng	(177)			
2		VDIVDRFAHF	LPIKVICELL	GVD-----	EAARGAF	GRWSSEILvm	(177)			
3		CDEMDCALY	YPLHVMTAL	GVE-----	EDDEFLM	LKLTODEfgv	(190)			
4		CNETDYAEP	EPILBFMLIA	GVE-----	EDDIPHL	KYLTDOMtrp	(187)			
5		LEVPEDMTRL	TLDITGLCGE	NYRfnsfyrd	qphPFTSMV	RALDEAMNkl	(188)			
6		CDPTFILGCA	PCNVICSVIE	HNrfdyk--d	EEFLKIM	ESLHENVEll	(208)			
7		CDPTFILGCA	PCNVICSVIE	HNrfdyk--d	EEFLKIM	ESLHENVRil				
8		CDPTFLFCV	PCNVICSVIE	QNRfdyd--d	EKFKTLI	KYFHENFell				
9		CNPTFILGAA	PCNVICSVIE	QNRfdyt--d	QDFLSIM	GKLNENFKil				
10		VTMKKVFAY	SMDVITSTS	GVNvdsl--n	NPKDPFV	EKTKLLRfd				
11		VTLKDFVAY	SMDVITSTS	GVNvdsl--n	NPKDPFV	ENTKLLRfd				

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12	VTLKDVFGAY SMDVITSTSE GVN	idsl--n ---NEODPFV-ENTKKLLRfd	(213)
	CSB 3	CSB 4	
1	-----s stare	ASAAN OELDYLAILE VEORIV	(204)
2	d-----p eraeq	GOAA REVVNEILDL VERRRT	(205)
3	-----g sm--t	FAEAK EALYDYLFPI IEORRO	(213)
4	qra---npdd -pa---y-d	enkrqFOEDI KVMNDLVDKI IADRKas	(226)
5	gtpwlqvynn fpalldyfp	gihktLLKNA DYIKNFIMEK VKEHEKl	(256)
6	sspwlvqynn fpalldyfp	gihktLLKNA DYIKNFIMEK VKEHEKl	
7	gtpwqlyni fpl-lhylp	gshrqLFKNI DGQIKFILEK VQEHQEs	
8	nspwvqmcnn fpilidyfp	gshnkILRNN IYIRNYVLEK IKEHQEt	
9	ffd--pfls vvlfpfltpi	yemlnICMFP KDSIEFFKKF VYRMKEtrld	
10	fld--pfls itvfpflipi	levlnICVFP REVTFNLRKA VKRMKEsrle	
11	fld--pfls itvfpflipi	levlnICVFP REVTFNLRKS VKRMKEsrle	(261)
12		CSB 5	
1	---epkdDIT SKLCTeqvqp	--g-----nIDKSDAVOI AFILLVAGNA	(242)
2	---epgdDL SALLSvqddd	-dg-----rLSADELTST AIVLLAGFE	(244)
3	---cpkdDVM SLLANSkl-d	--gn-----yIDDKYINAY XVAIATAGHD	(270)
4	---kpgtDAI SIVANGqvn	--gr-----pITSDEAKRM CGILLVGGIL	(251)
5	---geqsDILL THMLngkdp	t-ge-----plDDENIRYO ITTFLIAGHE	(267)
6	-v-nnpDDEI DCFLLkmeqe	n-----l eftLESILVIA VSDLFAGTE	(297)
7	-v-nnpDDEI DCFLLkmeqe	n-----l eftLESILVIA VSDLFAGTE	
8	s-nnpDDEV DHFLIkmeqe	k-----hkkqs eftMDNLITT INDVFSAGHD	
9	-i-nnpDDEI DCFLLkmeqe	kd---nqq-s eftTIENLMTT LSDVFGAGTE	
10	svqkhrvDEL QLMNahnds	kdksht---alSDMEITAO SIIFIFAGYE	
11	dtqkhrvDEL QLMIDshkns	keteshk---alSDLELVAO SIIFIFAGYE	
12	dtqkhrvDEL QLMIDsq-ns	keteshk---alSDLELVAO SIIFIFAGYE	(307)
	CSB 6	CSB 7A	
1	TMVNIALGV ATTAC	HEDQ LAOLKA	-----npsIA (272)
2	ASVSLIGIGT YLLLT	HEDQ LAIVRA	-----dpsAI (274)
3	ITSSSSGGAT IGLSR	NEEO LALAKS	-----dpALI (300)
4	RVVNELSFEM EFLAK	SEEH ROELLE	-----rPERT (281)
5	ITSGLLSFAL YFLVK	NPHV LOKAAEd	aa rvlvdp-vgs ykqvklkv (314)
6	ITSTTLRYSL LLILK	HPEV AARVOEe	er vigrhrs-pc mqdrsrpvt (345)
7	ITSTTLRYSL LLILK	HPEV AARVOEe	er vigrhrs-pc mqdrsrpvt
8	ITSTTLRYSL LLILK	HPEI TAKVOEe	feh vigrhrs-pc mqdrtrpvt
9	ITSTTLRYGL LLILK	HPEV IAKVOEe	er vigrhrs-pc mqdrsrpvt
10	ITSSVLSFIM HSLAT	HEDT OKKLOEe	idr alpka-ppt ydtvmeqvl
11	ITSSVLSFIM YELAT	HEDV OOKLOEe	ida vlpnka-ppt ydtvlgmvl
12	ITSSVLSFIM YELAT	HEDV OOKLOEe	ida vlpnka-ppt ydtvlgmvl (355)
	CSB 7A	CSB 7B	CSB 8
1	POFVEELCRY HTASalaikr	TAKEDVMIGD	-KLVRANEGT IASNOANRD (321)
2	PNAVEELRY IAPPet-tr	FAAEVEIGG	-VAIPOYSTV LVANGAANRD (322)
3	PRLYDEAVRW TAPVks-fmr	TALADTEVRG	-ONIKRGDRI MLYPSANRD (348)
4	PAACEELLR FSLVa--dgr	ILTSDFYFHC	-VOLKRGDQI LIPOMISGLD (328)
5	GMVLNEALRL WPTAp-afst	TAKEDTVLGG	eYPLEKDEI MVLIPOLHRD (363)
6	DAVHEIORF IDLLptnlph	AVTRDVRFRN	-YFIKGTDI ITSLTSVLHD (394)
7	DAVHEIORF IDLLptnlph	AVTRDVRFRN	-YFIKGTDI ITSLTSVLHD
8	DAVMEIORY VDLVptslph	AVTDIEFNG	-YLIFKGTDI IPSLTSVLHD
9	DATVHEIORY INLIpnnvER	ATTGNVKFRS	-YLIFKGTAV ITSLTSMYLN
10	DMVLNETLRL YPIGnr-ler	VCKKQVEING	-VEMPKGSVV MIPSYALHRD
11	DMVNETLRL FPIAmr-ler	VCKKQVEING	-MFIKGGWV MIPSYALHRD
12	DMVNETLRL FPIAmr-ler	VCKKQVEING	-MFIKGGWV MIPSYALHRD (403)
	CSB 8	CSB 9	CSB 10
1	EEVE-ENFDE FNMmrk----	wppq-dp LGEGFGDHRG	IAEHLAKAET (362)
2	PSQE-PDFHR EDVtrd----	tr--gh LSFGQGIHFC	MGRPLAKLEG (361)
3	EEVE-SNEDE EDXtrf----	p-n-rh LGFGGGAHMC	LGOHLARLEM (387)
4	EREN-ACPMH VDEsrq----	k-v-sh ITTEGHCSHLG	LGOHLARLEI (367)
5	KLWDQDVEE TRPerfenps	a--ipqh-a KPEGNGORAC	IGQOFAHHA (410)
6	ERAT-FNEKV EDghfldes	-gnfkksdy MPESAGKMC	VGEGLARMEI (442)

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RESTRAINED DYNAMICS DOCKING OF
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7	EKAF-PNPKV	EDghfides	-gnfkksdyF	MPESAGKRC	VGEGLARMEL	
8	DKEF-PNPEK	EDghfides	-gnfkksdyF	MPESAGKRC	VGEGLARMEL	
9	DKEF-PNPD	EDghfildas	-gkfrksdyF	MPSTGKRC	VGEVLARMEL	
10	PQHW-PEPEE	EPERfsken	kgsidpy-vY	LPEGNCPNC	IGMRFALNM	
11	PKIW-TEPEK	ELERfskkn	kdnippy-iy	TEFGSGPNC	IGMRFALNM	(451)
12	PKYM-TEPEK	ELERfskkn	kdnidpy-iy	TEFGSGPNC	IGMRFALNM	

CSB 10 CSB 11 CSB 12A CSB 12B

1	TTVESTLYOK	E--PDLKvav	plgKINYTFL	NRdVGIVDLP	Vif	(403)
2	EVALRALFGR	EP-ALSLGid	ad-DVVWRRS	LILRGIDHL	Vrldg	(404)
3	KIFFEELUPK	I-kSVELsg	---PRLVAT	NEVGGPKNP	Irftka	(428)
4	IVTLKEWLTR	IpDFSIAE	g--AQIOHKS	GIvSGVOALP	Lvwdpattka v	(414)
5	TLVIGMMLKH	E--DFEDht	-n-YELDIKE	TLTLKPEGFV	Vkakskkipl gg	(457)
6	FLFLTSTLON	E--KLQSLve	pkdLITAVV	NGFVSVPPSY	Qlcf---ipi hh	(489)
7	FLFLTSTLON	E--KLQSLve	pkdLITAVV	NGFVSVPPSY	Qlcf---ipi	
8	FLFLTSTLON	E--TLKPLvd	pkdIDPTFVE	NGFVSVPPSY	Elcf-----	
9	FLFLTSTLON	E--TPKPLvd	pkdIDTFLV	SGIGRVPPLY	Qlsf-----	
10	KIATTKVLON	E--SFQPCke	tq-IPLKLSR	QGLOPTKPI	Ilkvvpr---	
11	KIATIRVLON	E--SEKPCke	tq-IPLKLSL	GGLOPEKPV	Vlkvesr---	
12	KIATIRVLON	E--SEKPCke	tq-IPLKLSL	GGLOPEKPV	Vlkvesrdgt vsga	(502)

CSB 12B CSB 13* CSB 13** CSB 13

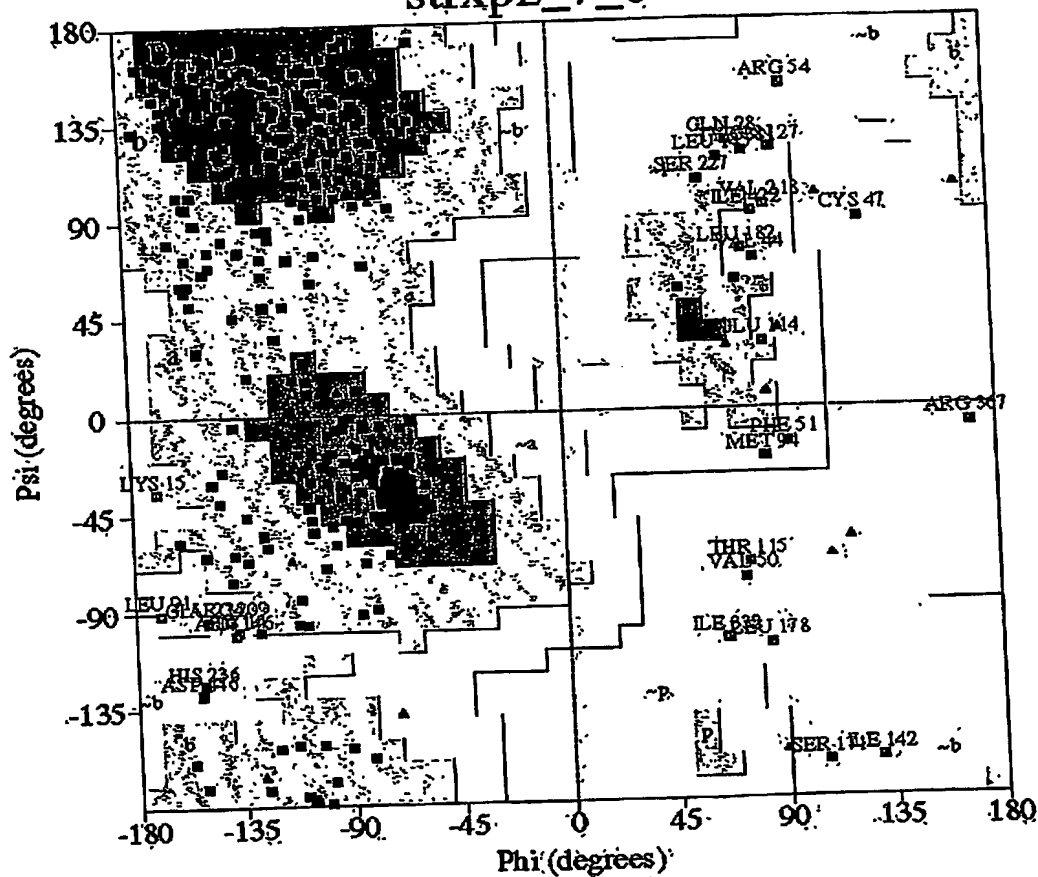
FIGURE 1

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PROCHECK

Ramachandran Plot

strxp2_7_0



Plot statistics

Residues in most favoured regions [A,B,L]	291	72.9%
Residues in additional allowed regions [a,b,l,p]	79	19.8%
Residues in generously allowed regions [-a,-b,-d,-p]	20	5.0%
Residues in disallowed regions:	9	2.3%
Number of non-glycine and non-proline residues	399	100.0%
Number of end-residues (excl. Gly and Pro)	2	
Number of glycine residues (shown as triangles)	21	
Number of proline residues	30	
Total number of residues	452	

FIGURE 2

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Appl. No.: Unassigned

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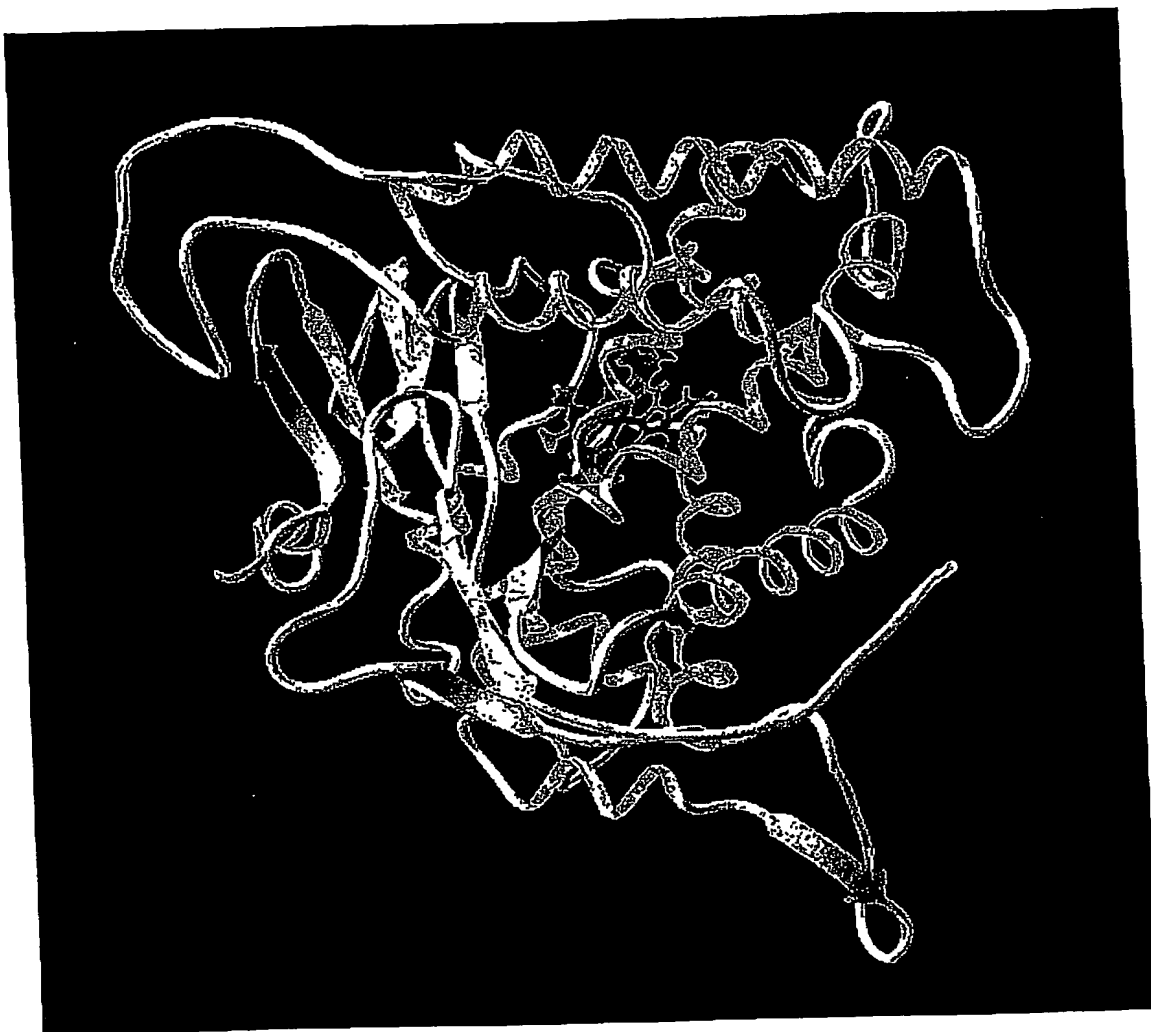


FIGURE 3

Title. A METHOD FOR PERFORMING
RESTRAINED DYNAMICS DOCKING OF
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Inventor(s): Francois Andre et al.
Appl. No.: Unassigned

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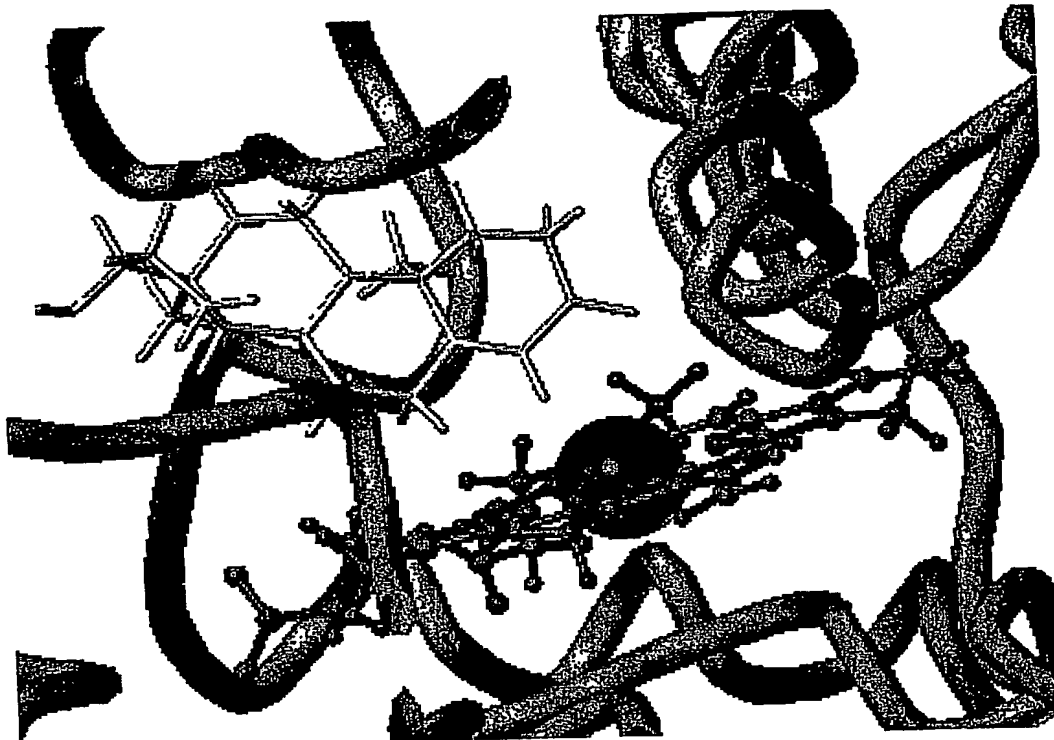


FIGURE 4

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Appl. No.: Unassigned

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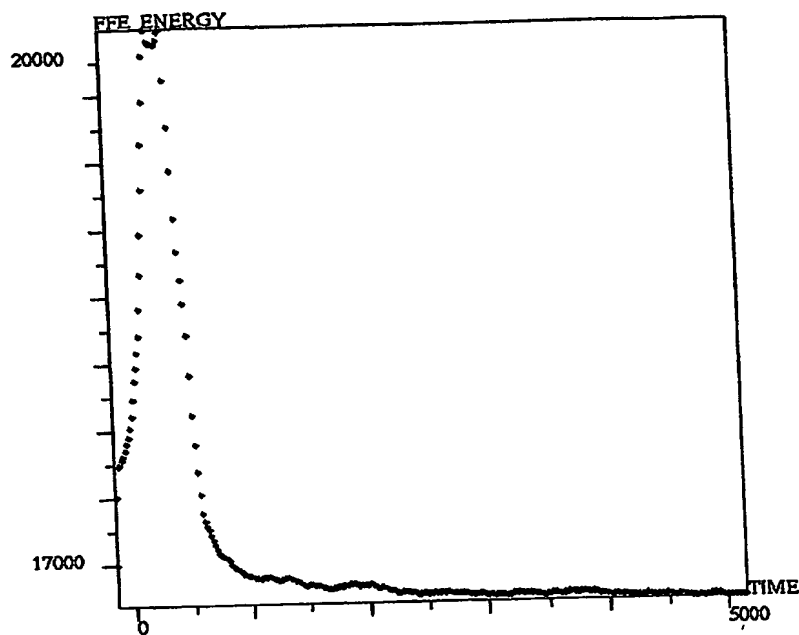


FIGURE 5